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Memorie della

Kurucz's WIDTH code and INPWIDTH

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Abstract. The WIDTH code written by R.L. Kurucz for abundance determination is here described in detail together with some changes that we made. The utility INPWIDTH code written by us to make easier the input for WIDTH is presented.

Key words. Stars: model atmospheres – Stars: Abundances

1. Introduction

WIDTH is a Fortran code written by R.L. Kurucz for the determination of the stellar abundances. They are derived by fitting the measured equivalent width W_m of single unblended lines to the computed equivalent width W_c. WIDTH is formed by the main program WIDTH, a set of subroutines belonging to WIDTH itself (LINCEN, WID, COG, AVERAG, VOIGT, and PLOTIT), and numerous subroutines belonging to the ATLAS code.

The WIDTH code was made public by Kurucz as version 5 in the years around 1970. The version number was related with the version 5 of the ATLAS code. The main program WIDTH and its own subroutines have not changed very much over the years, so that the successive versions, WIDTH6, WIDTH8, and WIDTH9 accounted mostly for the upgrades of the ATLAS code.

The last WIDTH9 version, together with some examples, are available at the Kurucz website[1]. Because, however, the documentation on WIDTH is rather scarce, in spite of this code is very old, we give some more details in this paper with the hope that they can be helpful for WIDTH users. In Sec. 5 we also present some changes that we made in the code, in particular an extension useful for deriving Mg abundance from the equivalent width of the Mg II triplet at 4481 Å. In Sec. 6 we describe the INPWIDTH code, an utility program written by us in order to avoid troubles related with the format for the input lines. The modified WIDTH9 version and the INPWIDTH code are available at our website[2]

2. The Theory

2.1. The computed equivalent width

The equivalent width

$$W_c = \int_{-\Delta\lambda}^{+\Delta\lambda} (1 - \frac{H_\nu(0)}{H_c(0)}) d\lambda$$

or

$$W_c = \int_{-\Delta\lambda}^{+\Delta\lambda} (1 - \frac{I_{\mu,\nu}(0)}{I_{\mu,c}(0)}) d\lambda$$

is computed in WIDTH by solving the half-integral from 0 to $\Delta\lambda$ by means of a sum over 15 points:

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[1] http://kurucz.harvard.edu/programs/width/

[2] http://wwwuser.oat.ts.astro.it/castelli/sources/width9.html

$$\frac{W_c}{2} = W = \sum_{i=1}^{15} w_i(1 - \frac{H_{\nu i}(0)}{H_{ci}(0)})$$

or

$$\frac{W_c}{2} = W = \sum_{i=1}^{15} w_i(1 - \frac{I_{\mu,\nu i}(0)}{I_{\mu,ci}(0)})$$

here $H_{\nu i}(0)$ and $H_{ci}(0)$ are the Eddington fluxes at the star surface (τ_ν=0). Their units are erg/cm^2/sec/hz/ster. Instead, $I_{\mu,\nu i}(0)$ and $I_{\mu,ci}(0)$ are the specific intensities at the surface for $\cos\theta=\mu$. They are required especially for the analysis of solar lines. The flux $H_{\nu i}(0)$ and the specific intensity $I_{\mu,\nu i}(0)$ are computed using both the opacity of the studied line and the continuous opacity, while $H_{ci}(0)$ and $I_{\mu,ci}(0)$ are the continuos flux and the continuous surface intensity computed using only the continuous opacities.

The weights w_i are the coefficients of the generalized Simpson rule:

$$\int_a^b f(x)dx =$$
$$h/3(f_1 + 4f_2 + f_3) + h/3(f_3 + 4f_4 + f_5) + ...$$

$$= h/3(f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5.....)$$

In WIDTH the actual width of the integration interval is h′=h SCALE, where h is the integration step listed in Table 1, col. 3. It is the difference between two successive intervals λ_i-$\lambda(0)$ (col. 2), where $\lambda(0)$ is the wavelength of the transition. The weights w_i are shown in col. 4.

SCALE is a scale factor related with the microturbulent velocity ξ. It is defined as:

$$SCALE = \frac{\sqrt{2.5^2+\Delta\lambda_{D\xi}^2}}{2.5}$$

where $\Delta\lambda_{D\xi}=(\xi/c)\lambda$. For ξ=0 km sec^{-1}, SCALE=1.

The scale factor SCALE is modified by iteration until the residual flux (residual intensity) at $\Delta\lambda$=5 SCALE is such that $0.91\leq H_\nu/H_c$ (I_ν/I_c) ≤ 0.93. SCALE increases or decreases the integration interval according to the extension of the line wings. Because

$$W_c=2W$$

the integration method adopted by WIDTH can be applied only to fully symmetrical profiles.

Table 1. Steps $\Delta\lambda$, their widths h, and the weights w_i for the integration over the line profile

i	λ_i-λ_0	h	w_i
	pm		
1	0		0.16667 (h/3)
		0.5	
2	0.5		0.66667 (4h/3)
		0.5	
3	1.0		0.33333 (2h/3)
		0.5	
4	1.5		0.66667
		0.5	
5	2.0		0.33333
		0.5	
6	2.5		0.66667
		0.5	
7	3.0		0.33333
		0.5	
8	3.5		0.66667
		0.5	
9	4.0		0.33333
		0.5	
10	4.5		0.66667
		0.5	
11	5.0		0.58333 (0.5+1.23/3)
		1.25	
12	6.25		1.66667 (4h/3)
		1.25	
13	7.5		0.83333 (2h/3)
		1.25	
14	8.75		1.66667
		1.25	
15	10.		0.41667 (h/3)

2.2. The computed Eddington fluxes and Specific Intensities

The computed continuous flux $H_c(0)$ and line flux $H_\nu(0)$ at the star surface (i.e. for τ_ν=0), are:

$$H_c(0) = \frac{1}{2}\int_0^\infty S_{\nu c}(t)E2(t)dt$$

$$H_\nu(0) = \frac{1}{2}\int_0^\infty S_{\nu l}(t)E2(t)dt$$

where the continuous source function $S_{\nu c}$ and the line source function $S_{\nu l}$ are given by:

$$S_{\nu c} = \frac{\sum_i \kappa_{\nu c}(i)S_{\nu c}(i)+\kappa_{\nu Hlin}(i)S_{\nu Hlin}(i)}{\sum_i \kappa_{\nu c}(i)+\kappa_{\nu Hlin}(i)}$$

$$S_{\nu l} = \frac{\sum_i \kappa_{\nu c}(i)S_{\nu c}(i)+\kappa_{\nu Hlin}(i)S_{\nu Hlin}(i)+\kappa_{\nu l}(i)S_l(i)}{\sum_i \kappa_{\nu c}(i)+\kappa_{\nu Hlin}(i)+\kappa_{\nu l}(i)}$$

The specific intensity for the line is:

$$I_{\mu,\nu}(0) = \int_0^\infty S_{\nu l} e^{\tau_{\nu l}/\mu} d\tau_{\nu l}/\mu$$

while that for the continuum is:

$$I_{\mu,c}(0) = \int_0^\infty S_{\nu c} e^{\tau_{\nu c}/\mu} d\tau_{\nu c}/\mu$$

The surface fluxes, the surface specific intensities, the source functions, the continuos absorption coefficient $\kappa_{\nu c}$, and the line opacity due to the wings of the hydrogen lines $\kappa_{\nu Hlin}$, are computed by means of the ATLAS subroutines.

2.3. The line absorption coefficient $\kappa_{\nu l}$ of the studied line

The line absorption coefficient is mostly computed by means of the subroutines belonging to the WIDTH code. It is:

$$\kappa_{\nu l} = \kappa_\nu(0) V(\alpha, \mathrm{v})(1 - e^{-h\nu/kT})$$

where $\kappa_\nu(0)$ is the absorption coefficient at the center of the line:

$$\kappa_\nu(0) = \frac{1}{\rho}\frac{\pi e^2}{m_e c} f_{ij} \frac{g_i N_J}{U_j} e^{-\chi_i/kT}$$

and V(v,α) is the Voigt function for the line profile.

$$V(\mathrm{v}, \alpha) = \frac{1}{\sqrt{(\pi)}\Delta\nu_D} H(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma}{4\pi\Delta\nu_D})$$

Therefore, the line absorption coefficient is:

$$\kappa_{\nu l} = \frac{1}{\rho}\frac{\pi e^2}{m_e c} f_{ij} \frac{g_i N_J}{U_j} e^{-\chi_i/kT} \frac{1}{\sqrt{(\pi)}\Delta\nu_D} H(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma}{4\pi\Delta\nu_D})(1 - e^{-h\nu/kT})$$

The Doppler shift, related with the Doppler line broadening, is

$$\Delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2kT}{\mu m_H} + \xi^2}$$

or

$$\Delta\lambda_D = \frac{c}{\lambda^2}\Delta\nu_D$$

The total damping constant γ is the sum:

$$\gamma = \gamma_r + \gamma_S + \gamma_{vW}$$

where γ_r, γ_S, and γ_{vW} are the radiative, Stark, and van der Waals damping constants, respectively.

Input data to compute the line absorption coefficient are: the microturbulent velocity ξ, log $g_i f_{ij}$, the excitation potential of the lower level χ_{lowi}, the damping constants, γ_r, γ_S/N_e, and γ_{vW}/N_H for T=10000 K. Here, N_e is the electron density and N_H is the neutral hydrogen density.

The elemental number density over the partition function N_j/U_j is computed with the ATLAS subroutines.

2.4. The Damping Constants γ_r, γ_S, γ_{vW}

The damping constants, as used in WIDTH and reported here, are described in Kurucz & Avrett (1981)

We note that the ionization potentials which are given in the WIDTH main program as a block of data are only used for computing damping constants and not for computing atomic number densities for which the ATLAS subroutines are used.

2.4.1. The radiative damping constant γ_r

When the radiative damping constant γ_r is not available from the literature, the classical value is assumed:

$$\gamma_r = 2.223 10^{13}/\lambda^2 \text{ for } \lambda \text{ in nm}$$

2.4.2. The Stark damping constant γ_s/N_e

When the Stark damping constant γ_S/Ne is not available from the literature, it is computed by the approximation:

$$\gamma_s/N_e = 10^{-8} n_{eff}^5$$

which is a fit by Peytremann (1972) to detailed calculations by Sahal-Brechot & Segre (1971). Here, n_{eff} is the effective quantum number of the upper state.

$$n_{eff}^2 = \frac{R Z_{eff}^2}{\chi_{ion} - \chi_{upper}}$$

where R=13.595 eV is the Rydberg energy, Z_{eff} is the effective charge (=1 for Fe I, 2 for Fe II, etc.), χ_{ion} is the ionization potential, and χ_{up} is the excitation potential of the upper level. If the upper level is above the ionization potential, because it ionizes to an excited level of the parent, n_{eff} is set to 5. For molecules, γ_s/Ne was arbitrarily assumed equal to 10^{-5}.

If γ_s is derived from the w half-half width listed by Griem (1975) it has the form:

$$\gamma_s/N_e = \frac{2\pi c(2W)}{\lambda_0^2}\frac{1}{Ne}$$

where Ne=10^{16} for neutral atom and Ne=10^{17} for ions. It follows that for neutral atoms:

$$\gamma_s/N_e = \frac{3767.3W}{\lambda_0^2}$$

and for ions:

$$\gamma_s/N_e = \frac{376.73W}{\lambda_0^2}$$

Usually, w values from Griem (1975) in the Kurucz's line lists are for T=10000 K.

2.4.3. The van der Waals damping constant γ_{vW}

The van der Waals damping constant γ_{vW} is computed with the classical formula (Aller 1963):

$$\gamma_{vW} = 17C_6^{2/5}\mathrm{v_i}^{3/5}Ni$$

where v_i is the mean velocity of the perturber with mass m_i relative to the radiator with mass m_{at}:

$$\mathrm{v_i} = \sqrt{\frac{8kT}{\pi}(1/m_{at} + 1/m_i)}$$

Possible perturbers are H I, He I, and H_2. Because $m_{at}=\mu$ M, where M=1.6598 10^{-24} gr is the atomic mass unit, and μ is the atomic weight, we obtain:

$$\mathrm{v_i} = \sqrt{\frac{8kT}{\pi M}(1/\mu_{at} + 1/\mu_i)}$$

Values for μ_i are 1 for hydrogen, 4 for helium, 2 for H_2.

The C_6 constant is given by:

$$C_6 = [\alpha_i(e^2/h)a_0^2\,|\Delta r^2|]^{0.4}$$

where e^2/h=34.836 10^6, a_0^2=2.8 10^{-17} cm^2 (Bohr radius), and α_i is the polarizability, which is 6.63 10^{-25} for H, 2.07 10^{-25} for He, and 8.04 10^{-25} for H_2. Furthermore:

$$|\Delta r^2| = |<r_{low}^2> - <r_{up}^2>|$$

where $<r_{low}^2>$ and $<r_{up}^2>$ are the mean square radii of the lower and upper levels, respectively. Combining the above formulas, and assuming μ_{at}>> 4 and r_{low}^2<< r_{up}^2 we get:

$$\gamma_H = 17[8kT/\pi M]^{0.3}\\ [6.63\ 10^{-25}e^2/h < r_{up} >^2 a_0^2]^{0.4}N_H$$

$$\gamma_{He} = 17[8kT/\pi M]^{0.3}(1/4)^{0.3}\\ [2.0710^{-25}e^2/h < r_{up} >^2 a_0^2]^{0.4}N_{He}$$

$$\gamma_{H2} = 17[8kT/\pi M]^{0.3}(1/2)^{0.3}\\ [8.0410^{-25}e^2/h < r_{up} >^2 a_0^2]^{0.4}N_{H2}$$

The sum of the γ's is:

$$\gamma_{vW} = 17[8kT/\pi M]^{0.3}[6.6310^{-25}(e^2/h)a_0^2]^{0.4}\\ (< r_{up} >^2)^{0.4}[N_H + 0.42N_{He} + 0.85N_{H2}]$$

After substitution of the constants it is:

$$\gamma_{vW} = 4.5\ 10^{-9}(< r_{up} >^2)^{0.4}\\ [N_H + 0.42N_{He} + 0.85N_{H2}](T/10000)^{0.3}$$

where

$$\gamma_{vW}/N_H = 4.5\ 10^{-9}\ \ < r_{up}^2 >^{0.4} \text{ for T = 10000 K}$$

The coefficient γ_{vW}/N_H for T=10000 K is either specified in input, or calculated. If it is NOT specified in input, it is computed from the following approximate expressions for $<r_{up}^2>$:

- For the iron group elements, i.e. for 20 < S < 29, where S is the atomic number:

  $$< r_{up} >^2 = (45 - S)/Z_{eff}$$

  This expression is the result of a fit to $<r_{up}^2>$ computed values obtained from 4p wavefunctions calculated by Kurucz, under the assumption that strong lines of the iron group elements have a 4p upper level. However, nowadays this approximation will be seldom used. In fact, γ_{vW}/N$_H$ is given for all the lines of the iron group included in the Kurucz line lists.

- For other atoms, the approximate formula valid for hydrogen-like levels of many light atoms is used:

$$< r_{up} >^2 \simeq 2.5(n_{eff}^2/Z_{eff})^2$$

- If the upper level is above the ionization potential (autoionization lines)

$$< r_{up}^2 >= 25.$$

- For molecules:

$$\gamma_{vW}/N_H = 1.0\ 10^{-7}/Z_{eff}$$

where the constant is arbitrarily adopted.

2.5. The Fitting Procedure

The line absorption coefficient for unit abundance $\overline{\kappa_{\nu l}}=\kappa_{\nu l}/\epsilon$(iz) is firstly computed for the ϵ abundance of the iz element read from the input model. It is then multiplied by different abundances which, starting from the initial value, are iteratively increased or decreased until to find that abundance for which |logW$_m$−logW$_c$| <0.005, where W$_m$ and W$_c$ are the measured and the computed equivalent widths.

Together with the equivalent widths W$_c$, the residual flux H$_\nu$/H$_c$ (or the residual specific intensity I$_{\mu,\nu}$/I$_{\mu,c}$) and the mean mass depth $(\rho$x$)_{av}$ at τ_ν=1, are also computed.

The mean mass depth $(\rho$x$)_{av}$ is defined as:

$$log_{10}(\rho x)_{av} = \frac{\int_0^b log_{10}(\rho x)_{\tau\nu=1}(1-H_\nu(0)/H_c(0))d\lambda}{\int_0^b (1-H_\nu(0)/H_c(0))d\lambda}$$

The integral is solved by means of the sum:

$$log_{10}(\rho x)_{av} = \frac{\sum_{i=0}^{15} w_i log_{10}(\rho x)_{\tau\nu=1}(1-H_\nu(0)/H_c(0))}{\sum_{i=1}^{15} w_i(1-\frac{H_{\nu i}}{H_{ci}})}$$

where w$_i$ are the integration weights given in Table 1.

Finally:

$$(\rho x)_{av} = 10^{log_{10}(\rho x)_{av}}$$

If residual specific intensities are considered, H$_\nu$(0) and H$_c$(0) are replaced by I$_{\mu,\nu}$(0) and I$_{\mu,c}$(0).

3. Subroutines in WIDTH

The WIDTH main program reads the input data and calls soubroutines for computing atomic and molecular number densities, continuous opacities, continuous surface fluxes or surface intensities, line absorption coefficients, line profiles, and equivalent widths. While most of the subroutines are those belonging to the ATLAS code, a few subroutines are part of WIDTH itself. They are:

```
LINCEN
WID
COG
AVERAG
VOIGT
PLOTIT
```

The subroutine LINCEN computes the line absorption coefficient in the line center for unit abundance $\overline{\kappa_\nu(0)}=\kappa_\nu(0)/\epsilon$(iz), the total damping constant γ, and the Doppler shift given both as $\Delta\nu_D$ and $\Delta\lambda_D$ (Sec. 2.3, 2.4, and 2.5).

We note that in WIDTH collisions with H_2 are assumed to be zero when γ_{vW} is computed, in that the H_2 molecular number density is set to zero in LINCEN.

The subroutine WID computes the equivalent widths by integrating over the profiles (Sec. 2.1).

The subroutine COG compares the measured equivalent width W$_m$ with the computed equivalent widths W$_c$ obtained for the different abundances, until to obtain |logW$_c$-logW$_m$|< 0.005 (Sec. 2.5).

Depending on the options given in input, COG may also compute a curve of growth, namely equivalent widths as function of abundances fixed at selected steps.

The subroutine AVERAG computes the average abundance with the mean square error from more different lines of the same ion. It also gives the slope of two straight lines of best fit: (1) excitation potentials of the lower level χ_{lowi} versus abundances logϵ_i, (2) computed equivalent widths W_{ci} versus abundances logϵ_i. The results from AVERAG are printed in form of plots by the subroutine PLOTIT which also shows the mass depths log$(\rho x)_i$ at τ_ν=1 versus abundances logϵ_i.

The subroutine VOIGT computes the part H(v,α) of the Voigt function V(v,α)(sec.2.3). The original Kurucz version of WIDTH makes use of a subroutine from Peytremann et al. (1967).

4. INPUT for WIDTH

Input for WIDTH are control cards, line data, and the model atmosphere. **The whole input ends with the STOP control card.**

4.1. Specific Control Cards for WIDTH

The specific control cards for WIDTH, which are read from unit 5, are:

```
VTUR
LINE
CURV
AVER
PROF
END
```

Their meaning together with examples of their use are given in Appendix A.

4.2. Input related with the Model Atmosphere

The input related with the model atmosphere is: (a) the input model, (b) the END control card

4.2.1. The input model

The model atmosphere can be entered either by assigning the model file to unit 3 and putting the control card:

READ PUNCH model-filename

or it can be entered directly, by putting the whole model atmosphere after the END control card, so that it will be read from unit 5.

4.3. ATLAS control cards useful for WIDTH

MOLECULES ON
READ MOLECULES

These two control cards have to be used if molecules contribute to the state equation. In this case, the file MOLECULES.DAT must be assigned to unit 2.

SURFACE INTENSITY 1 1.

It has to be used if the observed spectrum is an intensity spectrum instead of a flux spectrum. The first 1 indicates that only one cosθ is considered, the second value indicates that it is cosθ=1. This case holds for a spectrum observed in the center of the stellar disk. The default is SURFACE FLUX

OPACITY ON HLINES

This card must follow the OPACITY IFOP card of the input model. In this case, the wings of hydrogen lines with n < 5, where n is the quantum number of the lower level, contribute to the computed continuous opacity. Thanks to this option, abundances can be derived from lines lying on the far wings of the hydrogen lines, which should be considered as pseudo-continuum in the observed spectrum.

All the options related with the input model atmosphere can be modified by means of the same control cards used in ATLAS. For instance, abundances can be changed by using the cards:

ABUNDANCE CHANGE iz xabund(iz)

4.3.1. The END control card

It ends the input related with the model atmosphere. It has the form: END

5. A modified WIDTH version

We both did a few changes in the original Kurucz version of WIDTH and extended the code for deriving Mg abundance also from the measured equivalent width of the Mg II triplet at 4481 Å. The modified WIDTH version is available at our website[3].

5.1. The changes

1. We changed the convergence criterion from $|\log W_c - \log W_m| < 0.005$ to $|\log W_c - \log W_m| < 0.0005$.

2. We computed H(v,α) (Sec. 2.3) by means of a subroutine that interpolates for $v=\Delta\nu/\Delta\nu_D$ in the Harris (1948) tables, as it is done in SYNTHE. The original WIDTH code uses a different subroutine, which is from Peytremann et al. (1967). We did this change to be consistent with SYNTHE. However, some tests have shown that the two different methods do not give different results.

3. We modified the code so that van der Waals damping broadening from Baklem et al. (2000) can be used. A variable *alph* in the second data card after the LINE control card was added. If *alph*=0 the dependence of the van der Waals broadening on temperature goes as $T^{0.3}$, as before (Sect. 2.4.3). If *alph*=α, where α is taken from Barklem et al. (2000) tables, the dependence on temperature goes as $T^{(1-\alpha)/2}$. In this case, $\log_{10}(\gamma_{vW}/N_H)$ is taken from Barklem et al. (2000).
4. We compared the ionization potentials (in eV) given in the WIDTH main program as a block of data with those from Cowley et al. (2003) and, when different, we adopted the values from the Cowley et al. (2003) compilation. To convert from wavenumber to energy we adopted the relation 1eV=8065.545 cm^{-1}
   We would like to stress that updating these ionization potentials does not affect the accuracy of the abundances very much, because they are used only for computing approximate Stark and van der Waals broadening constants. Ionization potentials (in cm^{-1}) for computing atomic number densities are updated values stored in the IONPOTS subroutine of ATLAS

5.2. Mg abundance from the measured equivalent width of Mg II 4481 Å

The Mg II line at 4481.2 Å is a triplet whose components lie at 4481.126, 4481.150, and 4481.325 Å. Therefore, the observed line is a blend of the three components and could not be used in WIDTH to derive the Mg abundance.

We modified WIDTH in order to remove this drawback. The only condition is that of setting the input wavelength wl in the LINE cards equal to 448.12. In this case, the line absorption coefficients $\kappa_{\nu l}$ of the three components are separately computed at steps of 0.1 pm (0.01 Å) from $\lambda_0 - \lambda = -30$ pm (−3.0 Å) to $\lambda_0 + \lambda = +30$ pm (+3.0 Å), where $\lambda_0 = 448.12$ nm. At each step the three $\kappa_{\nu l}$ are summed together to produce the total line absorption coefficient at that wavelength. To get the total line profile a generalized Simpson rule with appropriate weights for the adopted step sizes was used. In order to compute the line profile and the equivalent width of Mg II 4481.2 Å, new subroutines COGmg, WIDmg, and LINCENmg were added in WIDTH. Kinman et al. (2000) derived the magnesium abundance from the equivalent width of Mg II 4481 Å in a sample of BHB star candidates by using this modified WIDTH version.

Such a procedure can be extended to other blended lines when the components are of the same species.

6. The INPWIDTH code

INPWIDTH is an interactive code written by us which generates input files for WIDTH without to be worried about their format. This

[3] http://wwwuser.oat.ts.astro.it/castelli/sources/width9.html

code is available at our website[4]. It can be compiled under LINUX equipped with the INTER-Fortran compiler by the command:

```
ifort -save -o inpwidth.exe inpwidth.for
```

The file inpwidth.com for executing INPWIDTH under LINUX is:

```
ln -s ~/lines/gf0100.100  fort.10
ln -s ~/lines/gf0150.100  fort.11
ln -s ~/lines/gf0200.100  fort.12
ln -s ~/lines/gf0300.100  fort.13
ln -s ~/lines/gf0400.100  fort.14
ln -s ~/lines/gf0500.100  fort.15
ln -s ~/lines/gf0600.100  fort.16
ln -s ~/lines/gf0800.100  fort.17
ln -s ~/lines/gf1200.100  fort.18
~/width/inpwidth.exe
mv fort.1 inpwidth.dat
rm fort.*
```

The gfxxxx.100 files are the line data from Kurucz's website or user's data with the same format. To execute INPWIDTH the command is:

source inpwidth.com

The code asks questions that have to be answered by the user. The only strong condition is that the wavelength given in input is exactly the same as in the input line lists.
The output file inpwidth.dat is the input for WIDTH. In this case, the command to execute WIDTH under LINUX is:

source width9.com

where width9.com is:

/width/width9.exe<inpwidth.dat>width.out

Results from WIDTH are in the file width.out. INPWIDTH generates also the file inplines.dat, where the line data are saved as they were typed by the user. This file can be used to add interactively more lines or to correct previous input data for a successive run of INPWIDTH.

[4] http://wwwuser.oat.ts.astro.it/castelli/sources/width/inpwidth.for

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Appendix A: Meaning and use of the WIDTH control cards

A.1. The **VTUR** *control card*

This control card should always be used !!!
It tells to the code to read the values for the microturbulent velocity ξ. It must be followed by a data card of the form:

nvt vts(1) vts(2) vts(3) [format(I5, 3F5.2)]

where nvt is the number of the constant microturbulent velocities ξ given in input (max 3) and vts(ivt) are the ξ values.

Caution: If nvt=1 and vts(1)=0, the code assumes as microturbulent velocity ξ that read from the input model (which can be different from 0!).

A.2. The **LINE** *control card*

It tells to the code to read the atomic (or molecular) data for the examined line. If the LINE control card does not come just after a CURV control card it gives rise to the fitting procedure for getting the required abundance (Sec. 2.5). It has the form:

LINE ew wlobs star [format(a4, f10.2, f10.4, 19a4)]

It must be followed by the two data cards:

1) wl gflog xj e xjp ep code label labelp
[format(f10.4, f7.3, f5.1, f12.3, f5.1, f12.3, f9.2, 2a4, a2, 2a4, a2)]

2) wl nelion gammar gammas gammaw ref nblo nbup iso1 x1 iso2 x2 other1 other2
[format(f10.4,i4,f6.2,f6.2,f6.2,a4,i2,i2,i3,f7.3,i3,f7.3,2a4,a2,2a4,a2)]

where:
ew=measured equivalent width in pm (1pm=10 mÅ, 10^{-2} Å)
wlobs=observed wavelength in nm (1nm=10^{-1}A) (may be blank)
star= the name of the star
wl=laboratory wavelength in nm
gflog=log gf
xj=J for the first energy level
e=first energy level in cm^{-1}
xjp=J for the second energy level
ep=second energy level in cm^{-1}
code=element code=element number+charge/100
label=label field for the first level (may be blank)
labelp=label field for the second level (may be blank)
nelion=(Z-1)*6+(charge+1) (i.e. Fe I⟶ nelion=(26-1)*6+1=151)
gammar=$\log_{10}\gamma_r$
gammas=$\log_{10}(\gamma_S/\mathrm{Ne})$
gammaw=$\log_{10}(\gamma_{vW}/\mathrm{N}_H)$ for T=10000 K
ref=reference
nblo=non-LTE level index for the first level (may be blank)

nbup=non-LTE level index for the second level (may be blank)
iso1=isotope number (may be blank)
x1=log isotopic abundance fraction (may be blank)
iso2=isotope number (may be blank)
x2=hyperfine component log fractional strength (may be blank)
other1=label field (may be blank)
other2=label field (may be blank)

Example:

```
LINE     0.701 313.0420  HD 125072
  313.0420 -0.168  0.5       0.000  0.5   31935.340     4.01
  313.0420  20  0.00 -5.80  0.00BIE  0 0  0  0.000  0  0.000
```

The output will be of the form:

```
  313.0420 -0.168  0.5       0.000  0.5   31935.340     4.01
  313.0420  20  0.00 -5.80  0.00BIE  0 0  0  0.000  0  0.000
  HD 125072                                                          313.0420  8.36 -5.80 -7.96 -1.34   0.70  -10.647
         VTURB  ABUND   -11.60   -11.10   -10.65   -10.60   -10.65
          0.00     EW   -1.075   -0.584   -0.153   -0.111   -0.154
                          0.08     0.26     0.70     0.77     0.70
               DEPTH    -1.30    -1.31    -1.34    -1.34    -1.34
```

The **first two lines** show the line data as they were given in input. **The third line** lists the star name, the observed wavelength (in nm) (313.0420), the damping constants, logγ_r (8.36), logγ_s/N$_e$ (−5.80), logγ_{vW}/N$_H$ for T=10000 K (−7.96), the mass depth log(ρx) at τ_ν=1, averaged over the profile (−1.34), the measured equivalent width in pm (0.70), and the resulting abundance log(N$_{elem}$/N$_{tot}$) (-10.647). **The last four lines** list the abundance steps log(N$_{elem}$/N$_{tot}$) adopted in the fitting procedure, the corresponding computed equivalent widths in log, the computed equivalent widths, and the mean mass depths log(ρx) at τ_ν=1.

A.3. The **AVER** *control card*

It tells to the code to compute the average abundance from more different lines of the same ion. These lines, given in LINE control cards, have to be included between two AVER control cards.

Example:

```
AVER
LINE     0.158 477.1747  HD 125072
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     2.441 906.2487  HD 125072
  906.2487 -0.456  0.0   60333.430  1.0   71364.900     6.00
  906.2487  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     2.188 911.1807  HD 125072
  911.1807 -0.298  2.0   60393.140  1.0   71364.900     6.00
  911.1807  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     0.305 960.3034  HD 125072
  960.3034 -0.896  0.0   60333.430  1.0   70743.950     6.00
  960.3034  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
AVER
```

In addition to the whole output related with the LINE control cards, the C I average abundance from the C I lines at 477.1747, 906.2487, 911.1807, 960.3034 nm is computed. Furthermore, there are plots of abundance logϵ vs. excitation potential of the lower level χ_{low}, abundance logϵ vs. equivalent width W_c, and abundance logϵ vs. height in the atmosphere, given as mean mass depth log(ρx) at τ_ν=1 (Sec. 2.5).
The output has the form:

```
 477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
 477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
 HD 125072                                                                477.1747  7.99 -5.34 -7.34 -0.87   0.16  -3.817
        VTURB  ABUND    -4.78    -4.28    -3.78    -3.82
         0.00     EW   -1.759   -1.260   -0.764   -0.801
                         0.02     0.05     0.17     0.16
              DEPTH    -0.86    -0.87    -0.87    -0.87


 906.2487 -0.456  0.0   60333.430  1.0   71364.900     6.00
 906.2487  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
 HD 125072                                                                 906.2487  7.43 -6.12 -7.59 -1.19  2.44  -3.987
        VTURB  ABUND    -4.78    -4.28    -3.98    -3.94    -3.78    -3.99
         0.00     EW   -0.332    0.136    0.390    0.429    0.501    0.388
                         0.47     1.37     2.45     2.69     3.17     2.44
              DEPTH    -1.11    -1.14    -1.19    -1.20    -1.23    -1.19


 911.1807 -0.298  2.0   60393.140  1.0   71364.900     6.00
 911.1807  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
 HD 125072                                                                 911.1807  7.43 -6.12 -7.59 -1.18  2.19  -4.195
        VTURB  ABUND    -4.78    -4.28    -4.17    -3.78    -4.19
         0.00     EW   -0.188    0.268    0.364    0.582    0.340
                         0.65     1.85     2.31     3.82     2.19
              DEPTH    -1.12    -1.17    -1.19    -1.28    -1.18


 960.3034 -0.896  0.0   60333.430  1.0   70743.950     6.00
 960.3034  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
 HD 125072                                                                960.3034  7.38 -6.16 -7.60 -1.14   0.30  -4.494
        VTURB  ABUND    -4.78    -4.49    -4.28    -3.78    -4.49
         0.00     EW   -0.797   -0.514   -0.308    0.156   -0.516
                         0.16     0.31     0.49     1.43     0.31
              DEPTH    -1.13    -1.14    -1.15    -1.19    -1.14

VTURB 0.000    HD 125072

 ***** THE ABUNDANCE FROM   4         6.00 LINES IS  -4.12+/- 0.25

    LOG ABUND VS. CHI
     SLOPE= 0.316E+02 PER EV USING    4 LINES
      7.49 . - - - - . - - - - . - - - - . - -X- - . -X- - - I - X - - . - - - -X. - - - - . - - - - . - - - - .
      7.34 .         .         .         .         .         I         .         .         .         .         .
      7.19 .         .         .         .         .         I         .         .         .         .         .
      7.04 .         .         .         .         .         I         .         .         .         .         .
      6.89 .         .         .         .         .         I         .         .         .         .         .
      6.74 .         .         .         .         .         I         .         .         .         .         .
      6.59 .         .         .         .         .         I         .         .         .         .         .
      6.44 .         .         .         .         .         I         .         .         .         .         .
      6.29 .         .         .         .         .         I         .         .         .         .         .
      6.14 .         .         .         .         .         I         .         .         .         .         .
      5.99 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
      5.84 .         .         .         .         .         I         .         .         .         .         .
      5.69 .         .         .         .         .         I         .         .         .         .         .
      5.54 .         .         .         .         .         I         .         .         .         .         .
      5.39 .         .         .         .         .         I         .         .         .         .         .
      5.24 .         .         .         .         .         I         .         .         .         .         .
      5.09 .         .         .         .         .         I         .         .         .         .         .
      4.94 .         .         .         .         .         I         .         .         .         .         .
      4.79 .         .         .         .         .         I         .         .         .         .         .
      4.64 .         .         .         .         .         I         .         .         .         .         .
```

```
        4.49 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        4.34 .         .         .         .         .         I         .         .         .         .         .
        4.19 .         .         .         .         .         I         .         .         .         .         .
        4.04 .         .         .         .         .         I         .         .         .         .         .
        3.89 .         .         .         .         .         I         .         .         .         .         .
        3.74 .         .         .         .         .         I         .         .         .         .         .
        3.59 .         .         .         .         .         I         .         .         .         .         .
        3.44 .         .         .         .         .         I         .         .         .         .         .
        3.29 .         .         .         .         .         I         .         .         .         .         .
        3.14 .         .         .         .         .         I         .         .         .         .         .
        3.00 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        2.85 .         .         .         .         .         I         .         .         .         .         .
        2.70 .         .         .         .         .         I         .         .         .         .         .
        2.55 .         .         .         .         .         I         .         .         .         .         .
        2.40 .         .         .         .         .         I         .         .         .         .         .
        2.25 .         .         .         .         .         I         .         .         .         .         .
        2.10 .         .         .         .         .         I         .         .         .         .         .
        1.95 .         .         .         .         .         I         .         .         .         .         .
        1.80 .         .         .         .         .         I         .         .         .         .         .
        1.65 .         .         .         .         .         I         .         .         .         .         .
        1.50 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        1.35 .         .         .         .         .         I         .         .         .         .         .
        1.20 .         .         .         .         .         I         .         .         .         .         .
        1.05 .         .         .         .         .         I         .         .         .         .         .
        0.90 .         .         .         .         .         I         .         .         .         .         .
        0.75 .         .         .         .         .         I         .         .         .         .         .
        0.60 .         .         .         .         .         I         .         .         .         .         .
        0.45 .         .         .         .         .         I         .         .         .         .         .
        0.30 .         .         .         .         .         I         .         .         .         .         .
        0.15 .         .         .         .         .         I         .         .         .         .         .
        0.00 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
          -3.12     -3.32     -3.52     -3.72     -3.92     -4.12     -4.32     -4.52     -4.72     -4.92     -5.12

VTURB 0.000    HD 125072

     LOG ABUND VS. EQ. WIDTH
      SLOPE= 0.255E-01 PER PM USING    4 LINES
        2.44 . - - - - . - - - - . - - - - . - - - - . -X- - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        2.39 .         .         .         .         .         I         .         .         .         .         .
        2.34 .         .         .         .         .         I         .         .         .         .         .
        2.29 .         .         .         .         .         I         .         .         .         .         .
        2.25 .         .         .         .         .         I         .         .         .         .         .
        2.20 .         .         .         .         .         I   X     .         .         .         .         .
        2.15 .         .         .         .         .         I         .         .         .         .         .
        2.10 .         .         .         .         .         I         .         .         .         .         .
        2.05 .         .         .         .         .         I         .         .         .         .         .
        2.00 .         .         .         .         .         I         .         .         .         .         .
        1.95 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        1.90 .         .         .         .         .         I         .         .         .         .         .
        1.86 .         .         .         .         .         I         .         .         .         .         .
        1.81 .         .         .         .         .         I         .         .         .         .         .
        1.76 .         .         .         .         .         I         .         .         .         .         .
        1.71 .         .         .         .         .         I         .         .         .         .         .
        1.66 .         .         .         .         .         I         .         .         .         .         .
        1.61 .         .         .         .         .         I         .         .         .         .         .
        1.56 .         .         .         .         .         I         .         .         .         .         .
        1.51 .         .         .         .         .         I         .         .         .         .         .
        1.46 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        1.42 .         .         .         .         .         I         .         .         .         .         .
        1.37 .         .         .         .         .         I         .         .         .         .         .
        1.32 .         .         .         .         .         I         .         .         .         .         .
        1.27 .         .         .         .         .         I         .         .         .         .         .
        1.22 .         .         .         .         .         I         .         .         .         .         .
        1.17 .         .         .         .         .         I         .         .         .         .         .
        1.12 .         .         .         .         .         I         .         .         .         .         .
        1.07 .         .         .         .         .         I         .         .         .         .         .
        1.03 .         .         .         .         .         I         .         .         .         .         .
        0.98 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
        0.93 .         .         .         .         .         I         .         .         .         .         .
        0.88 .         .         .         .         .         I         .         .         .         .         .
        0.83 .         .         .         .         .         I         .         .         .         .         .
        0.78 .         .         .         .         .         I         .         .         .         .         .
        0.73 .         .         .         .         .         I         .         .         .         .         .
        0.68 .         .         .         .         .         I         .         .         .         .         .
```

```
  0.63 .         .         .         .         .         I         .         .         .         .         .
  0.59 .         .         .         .         .         I         .         .         .         .         .
  0.54 .         .         .         .         .         I         .         .         .         .         .
  0.49 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
  0.44 .         .         .         .         .         I         .         .         .         .         .
  0.39 .         .         .         .         .         I         .         .         .         .         .
  0.34 .         .         .         .         .         I         .         .         .         .         .
  0.29 .         .         .         .         .         I         .        X.         .         .         .
  0.24 .         .         .         .         .         I         .         .         .         .         .
  0.20 .         .         .         .         .         I         .         .         .         .         .
  0.15 .         .         .         .    X    .         I         .         .         .         .         .
  0.10 .         .         .         .         .         I         .         .         .         .         .
  0.05 .         .         .         .         .         I         .         .         .         .         .
  0.00 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
     -3.12     -3.32     -3.52     -3.72     -3.92     -4.12     -4.32     -4.52     -4.72     -4.92     -5.12

VTURB 0.000    HD 125072


     LOG ABUND VS. LOG HEIGHT
 -0.87 . - - - - . - - - - . - - - - . - -X- - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
 -0.88 .         .         .         .         .         I         .         .         .         .         .
 -0.88 .         .         .         .         .         I         .         .         .         .         .
 -0.89 .         .         .         .         .         I         .         .         .         .         .
 -0.90 .         .         .         .         .         I         .         .         .         .         .
 -0.90 .         .         .         .         .         I         .         .         .         .         .
 -0.91 .         .         .         .         .         I         .         .         .         .         .
 -0.92 .         .         .         .         .         I         .         .         .         .         .
 -0.92 .         .         .         .         .         I         .         .         .         .         .
 -0.93 .         .         .         .         .         I         .         .         .         .         .
 -0.94 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
 -0.94 .         .         .         .         .         I         .         .         .         .         .
 -0.95 .         .         .         .         .         I         .         .         .         .         .
 -0.95 .         .         .         .         .         I         .         .         .         .         .
 -0.96 .         .         .         .         .         I         .         .         .         .         .
 -0.97 .         .         .         .         .         I         .         .         .         .         .
 -0.97 .         .         .         .         .         I         .         .         .         .         .
 -0.98 .         .         .         .         .         I         .         .         .         .         .
 -0.99 .         .         .         .         .         I         .         .         .         .         .
 -0.99 .         .         .         .         .         I         .         .         .         .         .
 -1.00 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
 -1.01 .         .         .         .         .         I         .         .         .         .         .
 -1.01 .         .         .         .         .         I         .         .         .         .         .
 -1.02 .         .         .         .         .         I         .         .         .         .         .
 -1.03 .         .         .         .         .         I         .         .         .         .         .
 -1.03 .         .         .         .         .         I         .         .         .         .         .
 -1.04 .         .         .         .         .         I         .         .         .         .         .
 -1.04 .         .         .         .         .         I         .         .         .         .         .
 -1.05 .         .         .         .         .         I         .         .         .         .         .
 -1.06 .         .         .         .         .         I         .         .         .         .         .
 -1.06 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
 -1.07 .         .         .         .         .         I         .         .         .         .         .
 -1.08 .         .         .         .         .         I         .         .         .         .         .
 -1.08 .         .         .         .         .         I         .         .         .         .         .
 -1.09 .         .         .         .         .         I         .         .         .         .         .
 -1.10 .         .         .         .         .         I         .         .         .         .         .
 -1.10 .         .         .         .         .         I         .         .         .         .         .
 -1.11 .         .         .         .         .         I         .         .         .         .         .
 -1.12 .         .         .         .         .         I         .         .         .         .         .
 -1.12 .         .         .         .         .         I         .         .         .         .         .
 -1.13 . - - - - . - - - - . - - - - . - - - - . - - - - I - - - - . - - - - . - - - - . - - - - . - - - - .
 -1.13 .         .         .         .         .         I         .         .         .         .         .
 -1.14 .         .         .         .         .         I         .        X.         .         .         .
 -1.15 .         .         .         .         .         I         .         .         .         .         .
 -1.15 .         .         .         .         .         I         .         .         .         .         .
 -1.16 .         .         .         .         .         I         .         .         .         .         .
 -1.17 .         .         .         .         .         I         .         .         .         .         .
 -1.17 .         .         .         .         .         I         .         .         .         .         .
 -1.18 .         .         .         .         .         I         .         .         .         .         .
 -1.19 .         .         .         .         .         I   X     .         .         .         .         .
 -1.19 . - - - - . - - - - . - - - - . - - - - . -X- - - I - - - - . - - - - . - - - - . - - - - . - - - - .
     -3.12     -3.32     -3.52     -3.72     -3.92     -4.12     -4.32     -4.52     -4.72     -4.92     -5.12
```

A.4. The **CURV** control card

It tells to the program to compute up to a 9 points curve of growth. Namely, equivalent widths W_c(i) are computed for a given number (max 9) of abundances. At the same time, the corresponding reduced flux at the center of the line, $H_{\nu_i}(0)/H_{ci}(0)$ (or the reduced intensity at the center of the line $I_{\mu\nu_i}(0)/I_{\mu ci}(0)$), and the average mass depths $\log(\rho x)_i$ at τ_ν=1 are computed.

The CURV control card must be followed by a data card and by a LINE card. The data card which follows immediately the CURV control card has the form:

nablog minlog dablog [format(I5, 2F8.2)]

nablog is the number of points of the curve of growth. If nablog=0 no curve of growth is computed.
minlog is the scale factor (in log) to apply to the input abundance for the studied line in order to get the lowest abundance $\log\epsilon_{min}$ for the curve of growth.
dablog is the step (in log) of the logarithmic abundance $\log\epsilon$

Example:

```
CURV
    5   -1.0    0.5
LINE      0.158 477.1747  HD 125072
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
```

For an input carbon abundance $\log(N(C)/N_{tot})$=-3.78, the output has the form:

```
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
   HD 125072                                                      477.1747  7.99 -5.34 -7.34 -1.73    0.16   -0.780
        VTURB  ABUND    -4.78    -4.28    -3.78    -3.28    -2.78    -2.28    -1.78    -1.28    -0.78
         0.00     EW   -1.759   -1.260   -0.764   -0.278    0.184    0.522    0.804    0.986    1.111
                         0.02     0.05     0.17     0.53     1.53     3.33     6.36     9.69    12.91
               DEPTH    -0.86    -0.87    -0.87    -0.89    -0.93    -1.07    -1.28    -1.52    -1.73
               RESID     1.00     1.00     0.99     0.96     0.89     0.75     0.59     0.48     0.41
```

The meaning of this output is the same as that described for the LINE control card.

A.5. The **PROF** control card

It sets in the code the switch IPROF to 1 and produces the printout of 15 points half-profiles for all the lines of subsequent LINE control cards. The default is IPROF=0.

Example:

```
PROF
LINE      0.158 477.1747  HD 125072
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
```

The number of half-profiles in output is that of the abundances used to fit the measured equivalent width. The half-profiles are residual fluxes H_ν/H_c (or residual intensities $I_{\mu\nu}/I_{\mu c}$) at $\Delta\lambda$=h SCALE ($\Delta\lambda$ in pm, 1 pm=10 mÅ, 1 pm=10^{-2} Å) (Sec. 2.1).
The output is:

```
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
```

```
 PROFILES FOR NEXT LIN
         DEL  0.000  0.500  1.000  1.500  2.000  2.500  3.000  3.500  4.000  4.500  5.000  6.250  7.500  8.750 10.000
       DEPTH -0.876 -0.876 -0.876 -0.875 -0.875 -0.874 -0.874 -0.873 -0.872 -0.872 -0.871 -0.869 -0.867 -0.866 -0.865
       RESID  0.986  0.987  0.987  0.987  0.988  0.988  0.989  0.990  0.991  0.992  0.993  0.995  0.997  0.998  0.999
         DEL  0.000  0.500  1.000  1.500  2.000  2.500  3.000  3.500  4.000  4.500  5.000  6.250  7.500  8.750 10.000
       DEPTH -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.865 -0.864 -0.864
       RESID  0.999  0.999  0.999  0.999  0.999  0.999  0.999  0.999  0.999  0.999  0.999  0.999  1.000  1.000  1.000
         DEL  0.000  0.500  1.000  1.500  2.000  2.500  3.000  3.500  4.000  4.500  5.000  6.250  7.500  8.750 10.000
       DEPTH -0.868 -0.868 -0.868 -0.868 -0.868 -0.867 -0.867 -0.867 -0.867 -0.867 -0.866 -0.866 -0.865 -0.865 -0.865
       RESID  0.996  0.996  0.996  0.996  0.996  0.996  0.997  0.997  0.997  0.997  0.998  0.998  0.999  0.999  1.000
         DEL  0.000  0.500  1.000  1.500  2.000  2.500  3.000  3.500  4.000  4.500  5.000  6.250  7.500  8.750 10.000
       DEPTH -0.875 -0.875 -0.875 -0.875 -0.874 -0.874 -0.873 -0.872 -0.872 -0.871 -0.870 -0.869 -0.867 -0.866 -0.865
       RESID  0.988  0.988  0.988  0.988  0.989  0.989  0.990  0.991  0.992  0.992  0.993  0.995  0.997  0.998  0.999
 HD 125072                                                                477.1747  7.99 -5.34 -7.34 -0.87   0.16  -3.817
         VTURB  ABUND    -4.78    -4.28    -3.78    -3.82
          0.00     EW   -1.759   -1.260   -0.764   -0.801
                          0.02     0.05     0.17     0.16
                DEPTH    -0.86    -0.87    -0.87    -0.87
```

A.6. The **END** *control cards*

END ends the input related with the lines. After the END control card the input related with the model atmosphere starts.

Appendix B: An Example of command file

In what follows we give an example of command file to run WIDTH under LINUX. The whole input is read from unit 5, the output is the file width9.out.

```
ln -s ~/atlas9/molecules.dat fort.2
~/width/width9.exe<<EOF>width9.out
VTUR
    1 0.00  1.50  2.00
LINE     0.701 313.0420  HD 125072
  313.0420 -0.168  0.5       0.000  0.5   31935.340     4.01
  313.0420  20  0.00 -5.80  0.00BIE  0 0  0  0.000  0  0.000
LINE     1.070 345.1287  HD 125072
  345.1287  0.293  1.0   73396.600  2.0  102363.000     5.01
  345.1287  26  0.00  0.00  0.00NIST 0 0  0  0.000  0  0.000
AVER
LINE     0.158 477.1747  HD 125072
  477.1747 -1.866  2.0   60393.140  2.0   81343.990     6.00
  477.1747  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     2.441 906.2487  HD 125072
  906.2487 -0.456  0.0   60333.430  1.0   71364.900     6.00
  906.2487  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     2.188 911.1807  HD 125072
  911.1807 -0.298  2.0   60393.140  1.0   71364.900     6.00
  911.1807  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
LINE     0.305 960.3034  HD 125072
  960.3034 -0.896  0.0   60333.430  1.0   70743.950     6.00
  960.3034  31  0.00  0.00  0.00CNO  0 0  0  0.000  0  0.000
AVER
AVER
LINE     0.868 657.8052  HD 125072
  657.8052 -0.026  0.5  116537.650  1.5  131735.520     6.01
  657.8052  32  9.07 -5.35  0.00CNO  0 0  0  0.000  0  0.000
LINE     0.760 658.2882  HD 125072
  658.2882 -0.328  0.5  116537.650  0.5  131724.370     6.01
  658.2882  32  9.07 -5.35  0.00CNO  0 0  0  0.000  0  0.000
LINE     0.323 723.1333  HD 125072
  723.1333  0.043  0.5  131724.370  1.5  145549.270     6.01
  723.1333  32  0.00 -5.37  0.00CNO  0 0  0  0.000  0  0.000
LINE     0.908 723.6420  HD 125072
  723.6420  0.298  1.5  131735.520  2.5  145550.700     6.01
  723.6420  32  0.00 -5.37  0.00CNO  0 0  0  0.000  0  0.000
```

```
LINE     1.239 391.8968  HD 125072
  391.8968 -0.533  0.5  131724.370  0.5  157234.070     6.01
  391.8968  32  8.98 -4.93  0.00CNO  0 0  0  0.000  0  0.000
AVER
END
TEFF  12000.  GRAVITY 3.95000 LTE
TITLE ATLAS12
MOLECULES ON
READ MOLECULES
 OPACITY IFOP 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0
OPACITY ON HLINES
 CONVECTION ON   1.25 TURBULENCE OFF  0.00  0.00  0.00  0.00
ABUNDANCE SCALE   1.00000 ABUNDANCE CHANGE 1 0.97780 2 0.02090
 ABUNDANCE CHANGE  3 -10.90  4 -10.60  5  -9.45  6  -3.78  7  -4.08  8  -3.17
 ABUNDANCE CHANGE  9  -7.44 10  -3.92 11  -5.67 12  -4.81 13  -7.50 14  -4.45
 ABUNDANCE CHANGE 15  -6.55 16  -4.67 17  -6.50 18  -5.60 19  -6.88 20  -5.64
 ABUNDANCE CHANGE 21  -8.83 22  -5.52 23  -9.94 24  -5.47 25  -4.15 26  -4.84
 ABUNDANCE CHANGE 27  -7.08 28  -6.39 29  -7.79 30  -7.40 31  -5.16 32  -8.59
 ABUNDANCE CHANGE 33  -9.63 34  -8.59 35  -9.37 36  -8.69 37  -9.40 38  -8.54
 ABUNDANCE CHANGE 39  -6.90 40  -9.40 41 -10.58 42 -10.08 43 -19.96 44 -10.16
 ABUNDANCE CHANGE 45 -10.88 46 -10.31 47 -11.06 48 -10.23 49 -10.34 50 -10.00
 ABUNDANCE CHANGE 51 -11.00 52  -9.76 53 -10.49 54  -9.83 55 -10.87 56  -9.87
 ABUNDANCE CHANGE 57 -10.83 58 -10.42 59 -11.29 60 -10.50 61 -20.00 62 -10.99
 ABUNDANCE CHANGE 63 -11.49 64 -10.88 65 -11.65 66 -10.86 67 -11.74 68 -11.07
 ABUNDANCE CHANGE 69 -12.00 70 -10.92 71 -11.94 72 -11.12 73 -12.13 74 -10.89
 ABUNDANCE CHANGE 75 -11.72 76 -10.55 77 -10.65 78 -10.20 79 -10.99 80  -6.50
 ABUNDANCE CHANGE 81 -11.10 82 -10.05 83 -11.29 84 -20.00 85 -20.00 86 -20.00
 ABUNDANCE CHANGE 87 -20.00 88 -20.00 89 -20.00 90 -11.91 91 -20.00 92 -12.50
 ABUNDANCE CHANGE 93 -20.00 94 -20.00 95 -20.00 96 -20.00 97 -20.00 98 -20.00
 ABUNDANCE CHANGE 99 -20.00
 ABUNDANCE CHANGE  5 -6.45
 ABUNDANCE CHANGE 10 -4.92
 ABUNDANCE CHANGE 40 -8.80
 ABUNDANCE CHANGE 46 -6.51
 ABUNDANCE CHANGE 56 -9.27
 ABUNDANCE CHANGE 70 -7.35
READ DECK6 72 RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB
 3.54193513E-07   6510.4 3.080E-03 1.658E+09 3.766E-01 2.160E+02 0.000E+00 0.000E+00 0.000E+00
 4.72454749E-07   6535.8 4.107E-03 2.193E+09 3.757E-01 2.258E+02 0.000E+00 0.000E+00 0.000E+00
 6.30685157E-07   6555.8 5.481E-03 2.901E+09 3.741E-01 2.354E+02 0.000E+00 0.000E+00 0.000E+00
 8.42593895E-07   6582.3 7.318E-03 3.835E+09 3.726E-01 2.438E+02 0.000E+00 0.000E+00 2.747E+08
 1.12620824E-06   6615.8 9.775E-03 5.065E+09 3.715E-01 2.493E+02 0.000E+00 0.000E+00 2.312E+08
 1.50528674E-06   6654.0 1.306E-02 6.686E+09 3.709E-01 2.532E+02 0.000E+00 0.000E+00 1.900E+08
 2.01098358E-06   6698.7 1.743E-02 8.819E+09 3.712E-01 2.547E+02 0.000E+00 0.000E+00 1.549E+08
 2.68376682E-06   6748.9 2.326E-02 1.162E+10 3.724E-01 2.540E+02 0.000E+00 0.000E+00 1.237E+08
 3.57684313E-06   6803.5 3.099E-02 1.529E+10 3.747E-01 2.517E+02 0.000E+00 0.000E+00 9.733E+07
 4.75864429E-06   6862.1 4.123E-02 2.008E+10 3.781E-01 2.481E+02 0.000E+00 0.000E+00 7.557E+07
 6.31810578E-06   6923.3 5.474E-02 2.633E+10 3.827E-01 2.433E+02 0.000E+00 0.000E+00 5.772E+07
 8.37048372E-06   6985.7 7.253E-02 3.444E+10 3.883E-01 2.390E+02 0.000E+00 0.000E+00 4.366E+07
 1.10631193E-05   7049.3 9.589E-02 4.496E+10 3.951E-01 2.350E+02 0.000E+00 0.000E+00 3.280E+07
 1.45869887E-05   7113.8 1.265E-01 5.854E+10 4.032E-01 2.317E+02 0.000E+00 0.000E+00 2.449E+07
 1.91819956E-05   7179.6 1.664E-01 7.602E+10 4.130E-01 2.296E+02 0.000E+00 0.000E+00 1.826E+07
 2.51508824E-05   7248.5 2.182E-01 9.845E+10 4.250E-01 2.280E+02 0.000E+00 0.000E+00 1.358E+07
 3.28626591E-05   7321.4 2.852E-01 1.271E+11 4.398E-01 2.269E+02 0.000E+00 0.000E+00 9.991E+06
 4.27705363E-05   7399.3 3.712E-01 1.636E+11 4.579E-01 2.255E+02 0.000E+00 0.000E+00 7.200E+06
 5.54155002E-05   7483.0 4.811E-01 2.098E+11 4.799E-01 2.231E+02 0.000E+00 0.000E+00 5.001E+06
 7.14574636E-05   7571.6 6.205E-01 2.679E+11 5.060E-01 2.196E+02 0.000E+00 0.000E+00 3.296E+06
 9.16847740E-05   7664.2 7.964E-01 3.405E+11 5.363E-01 2.146E+02 0.000E+00 0.000E+00 2.075E+06
 1.17071759E-04   7758.8 1.017E+00 4.309E+11 5.711E-01 2.090E+02 0.000E+00 0.000E+00 1.239E+06
 1.48794314E-04   7853.7 1.294E+00 5.427E+11 6.106E-01 2.036E+02 0.000E+00 0.000E+00 7.205E+05
 1.88292999E-04   7948.2 1.638E+00 6.805E+11 6.553E-01 1.986E+02 0.000E+00 0.000E+00 4.029E+05
 2.37263474E-04   8042.1 2.064E+00 8.496E+11 7.060E-01 1.945E+02 0.000E+00 0.000E+00 2.171E+05
 2.97772389E-04   8135.2 2.592E+00 1.056E+12 7.635E-01 1.912E+02 0.000E+00 0.000E+00 1.169E+05
 3.72210503E-04   8227.8 3.241E+00 1.308E+12 8.289E-01 1.885E+02 0.000E+00 0.000E+00 6.275E+04
 4.63494896E-04   8319.8 4.038E+00 1.614E+12 9.033E-01 1.867E+02 0.000E+00 0.000E+00 3.342E+04
 5.74930002E-04   8411.3 5.010E+00 1.983E+12 9.881E-01 1.855E+02 0.000E+00 0.000E+00 1.752E+04
 7.10592357E-04   8502.2 6.194E+00 2.428E+12 1.085E+00 1.852E+02 0.000E+00 0.000E+00 8.884E+03
 8.75029302E-04   8592.2 7.630E+00 2.961E+12 1.195E+00 1.855E+02 0.000E+00 0.000E+00 4.215E+03
 1.07388482E-03   8681.2 9.364E+00 3.599E+12 1.320E+00 1.866E+02 0.000E+00 0.000E+00 1.694E+03
 1.31343419E-03   8768.3 1.145E+01 4.360E+12 1.463E+00 1.887E+02 0.000E+00 0.000E+00 3.690E+02
 1.60149870E-03   8853.5 1.397E+01 5.264E+12 1.625E+00 1.918E+02 0.000E+00 0.000E+00 0.000E+00
 1.94665301E-03   8936.5 1.698E+01 6.337E+12 1.809E+00 1.964E+02 0.000E+00 0.000E+00 0.000E+00
 2.35964086E-03   9017.9 2.057E+01 7.605E+12 2.020E+00 2.026E+02 0.000E+00 0.000E+00 0.000E+00
 2.85241932E-03   9098.2 2.487E+01 9.102E+12 2.259E+00 2.103E+02 0.000E+00 0.000E+00 0.000E+00
```

```
 3.43950048E-03   9178.0 2.997E+01 1.087E+13 2.530E+00 2.196E+02 0.000E+00 0.000E+00 0.000E+00
 4.13771878E-03   9257.9 3.604E+01 1.294E+13 2.839E+00 2.307E+02 0.000E+00 0.000E+00 0.000E+00
 4.96700869E-03   9338.5 4.323E+01 1.537E+13 3.189E+00 2.438E+02 0.000E+00 0.000E+00 0.000E+00
 5.95119380E-03   9420.9 5.176E+01 1.823E+13 3.586E+00 2.591E+02 0.000E+00 0.000E+00 0.000E+00
 7.11805273E-03   9506.8 6.184E+01 2.158E+13 4.034E+00 2.768E+02 0.000E+00 0.000E+00 0.000E+00
 8.50100016E-03   9598.6 7.377E+01 2.551E+13 4.539E+00 2.970E+02 0.000E+00 0.000E+00 0.000E+00
 1.01400733E-02   9699.1 8.787E+01 3.011E+13 5.106E+00 3.195E+02 0.000E+00 0.000E+00 0.000E+00
 1.20841492E-02   9811.2 1.046E+02 3.551E+13 5.738E+00 3.443E+02 0.000E+00 0.000E+00 0.000E+00
 1.43931357E-02   9938.1 1.243E+02 4.184E+13 6.435E+00 3.709E+02 0.000E+00 0.000E+00 0.000E+00
 1.71431818E-02  10083.1 1.478E+02 4.929E+13 7.192E+00 3.986E+02 0.000E+00 0.000E+00 0.000E+00
 2.04328301E-02  10250.3 1.757E+02 5.804E+13 7.995E+00 4.264E+02 0.000E+00 0.000E+00 0.000E+00
 2.43928022E-02  10443.7 2.093E+02 6.834E+13 8.824E+00 4.533E+02 0.000E+00 0.000E+00 0.000E+00
 2.92021338E-02  10667.8 2.499E+02 8.052E+13 9.644E+00 4.776E+02 0.000E+00 0.000E+00 0.000E+00
 3.51051083E-02  10927.3 2.996E+02 9.498E+13 1.041E+01 4.978E+02 0.000E+00 0.000E+00 0.000E+00
 4.24523709E-02  11227.2 3.614E+02 1.123E+14 1.107E+01 5.122E+02 0.000E+00 0.000E+00 0.000E+00
 5.17441014E-02  11572.5 4.394E+02 1.333E+14 1.158E+01 5.191E+02 0.000E+00 0.000E+00 0.000E+00
 6.37007034E-02  11970.0 5.397E+02 1.591E+14 1.190E+01 5.194E+02 0.000E+00 0.000E+00 0.000E+00
 7.93628005E-02  12428.2 6.712E+02 1.913E+14 1.201E+01 5.128E+02 0.000E+00 0.000E+00 0.000E+00
 1.00242187E-01  12953.1 8.467E+02 2.323E+14 1.192E+01 5.003E+02 0.000E+00 0.000E+00 0.000E+00
 1.28513612E-01  13555.8 1.085E+03 2.850E+14 1.167E+01 4.839E+02 0.000E+00 0.000E+00 0.000E+00
 1.67247508E-01  14245.2 1.412E+03 3.536E+14 1.130E+01 4.649E+02 0.000E+00 0.000E+00 0.000E+00
 2.20689661E-01  15023.3 1.864E+03 4.436E+14 1.091E+01 4.459E+02 0.000E+00 0.000E+00 0.000E+00
 2.94425004E-01  15901.2 2.489E+03 5.610E+14 1.057E+01 4.287E+02 0.000E+00 0.000E+00 0.000E+00
 3.95614622E-01  16872.4 3.348E+03 7.132E+14 1.030E+01 4.140E+02 0.000E+00 0.000E+00 0.000E+00
 5.33354833E-01  17943.6 4.519E+03 9.073E+14 1.014E+01 4.043E+02 0.000E+00 0.000E+00 0.000E+00
 7.19108703E-01  19117.8 6.100E+03 1.151E+15 1.008E+01 3.991E+02 0.000E+00 0.000E+00 0.000E+00
 9.66302337E-01  20396.1 8.205E+03 1.452E+15 1.015E+01 3.996E+02 0.000E+00 0.000E+00 0.000E+00
 1.29385115E+00  21795.1 1.099E+04 1.822E+15 1.020E+01 3.999E+02 0.000E+00 0.000E+00 0.000E+00
 1.73027900E+00  23312.4 1.471E+04 2.279E+15 1.018E+01 3.977E+02 0.000E+00 0.000E+00 0.000E+00
 2.31246089E+00  24964.0 1.967E+04 2.847E+15 1.022E+01 3.956E+02 0.000E+00 0.000E+00 0.000E+00
 3.08200875E+00  26743.8 2.622E+04 3.543E+15 1.035E+01 3.969E+02 0.000E+00 0.000E+00 0.000E+00
 4.08559774E+00  28681.7 3.476E+04 4.381E+15 1.069E+01 4.046E+02 0.000E+00 0.000E+00 0.000E+00
 5.36708235E+00  30764.7 4.566E+04 5.364E+15 1.127E+01 4.202E+02 0.000E+00 0.000E+00 0.000E+00
 6.97319105E+00  33030.3 5.928E+04 6.488E+15 1.209E+01 4.404E+02 0.000E+00 0.000E+00 0.000E+00
 8.95773990E+00  35462.7 7.610E+04 7.760E+15 1.312E+01 4.353E+02 0.000E+00 0.000E+00 0.000E+00
PRADK 2.7991E+01
BEGIN                   ITERATION  15 COMPLETED
END
STOP
EOF
rm fort.*
```