Hazy 1

a brief introduction to Cloudy

introduction and commands

version 08

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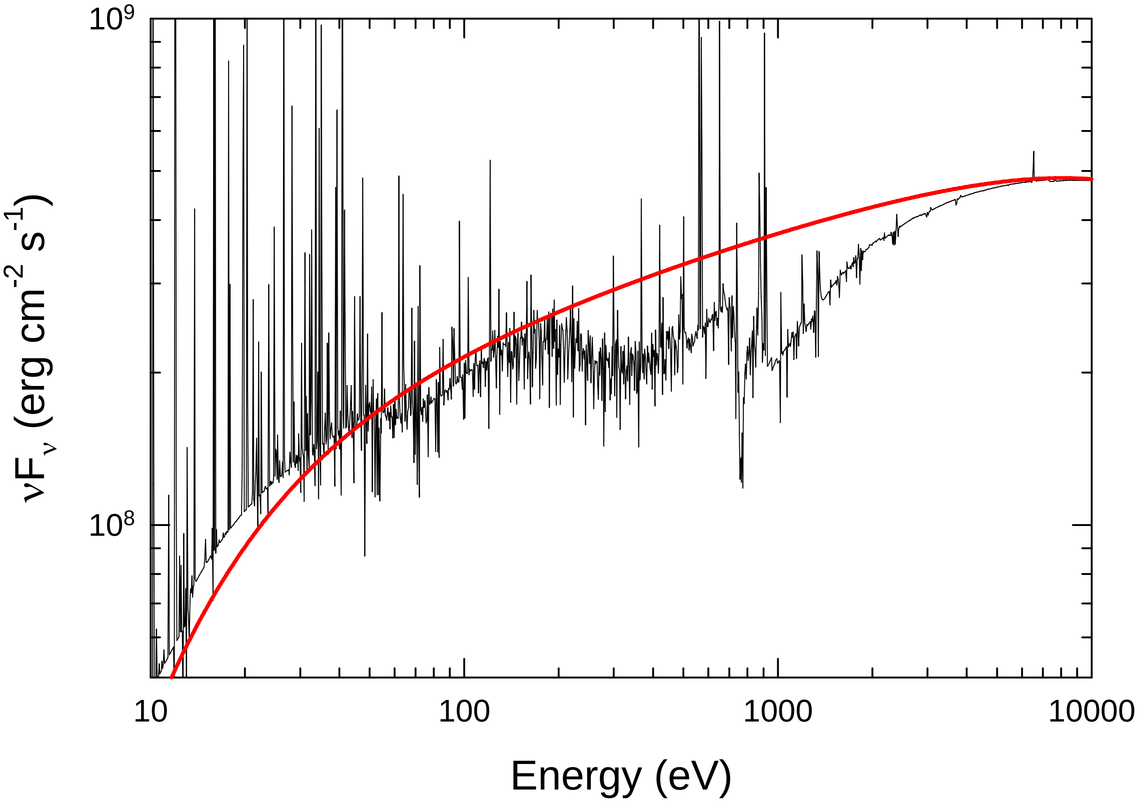

The predicted X-ray spectrum of a warm absorber in an Active Galactic Nucleus. Prominent emission and absorption lines are present along with broad UTA absorption features. The parameters are from Reynolds & Fabian (1995, MNRAS, 273, 1167)..

Use of this program is not restricted provided each use is acknowledged upon publication. The bibliographic reference to this version of Cloudy is "version xx.xx of the code last described by Ferland, G.J., et al 1998, PASP, 110, 761-778." The version number, shown here as "xx.xx", should be given and can be found on the first lines of the code's output.

Cloudy is an evolving code. You should confirm that you have the most recent version of the code by checking the web site http://www.nublado.org. The web site has a discussion board with emailing list. This will have announcements of any updates to the code.

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Cloudy 08

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1. INTRODUCTION

1.1. Overview

This describes the input, output, and assumptions for the spectral synthesis program Cloudy. It fully defines the commands used to drive the program. The methods, approximations, and assumptions used by Cloudy are outlined in Part 2 of this document, although this part, like Cloudy itself, is still under construction. Part 3 gives details about the program structure, its output, the computational environment, and how to call Cloudy as a sub-program of larger programs. The Quick Start guide summarizes these three volumes and gives a general overview of the simulations.

Many environments are encountered in which dilute gas is heated and ionized by the radiation field of a central object. Under these circumstances it is possible to predict the physical conditions (that is, the distribution of ionization, density, and temperature) across the cloud, and its resulting spectrum, in a unique and self-consistent manner. This is done by simultaneously solving the equations of statistical and thermal equilibrium, equations that balance ionization-neutralization processes, and heating-cooling processes, respectively. The graduate text Osterbrock & Ferland (2006, hereafter AGN3) describe the physics governing such environments. and Ferland (2003) provides additional details on current research topics in the physics of plasma emission.

1.2. What Cloudy can do

Cloudy is designed to simulate clouds ranging from the intergalactic medium to the high-density LTE limit. The range of temperatures and densities are described in detail in a section in Part 2 of this document. It predicts the thermal, ionization, and chemical structure of a cloud and its spectrum.

1.3. Setting up Cloudy

The instructions for setting up the code are on the web site http://www.nublado.org The web site includes a discussion board where questions can be posted.

1.4. What must be specified

One powerful asset of photoionization analysis is the large number of observables resulting from only a few input parameters. Intensities of many millions of spectral lines[1] are predicted by Cloudy. These result from the specification of only a) the shape and intensity of the external radiation field striking a cloud (referred to as the

[1] These is no limit to the number of spectral lines that the code can compute because there is no limit to the number of levels of atoms of the H-like (H^0, He^+, etc) and He-like (He^0, Li^+, etc) isoelectronic sequences. Processor speed and memory limit the simulation to a few million lines in most applications with today's computers, however.

incident continuum), b) the chemical composition and grain content of the gas, and c) the geometry of the gas, including its radial extent and the dependence of density on radius. The following subsections describe the general philosophy of the specification of each.

1.4.1. Incident continuum

Both the shape and intensity of the external continuum striking the cloud must be specified. Often this is the region's only source of heat and ionization. Different commands are usually used to specify the continuum shape and intensity, although a few commands specify both.

1.4.1.1. Continuum shape

The shape of the continuum should be fully specified between an energy of 1.001×10^{-8} Ryd ($\lambda \approx 10$ m) and an energy of 7.354×10^{6} Ryd ($h\nu \approx 100$ MeV) if possible. (In much of the following discussion photon energies will be given in Rydbergs. The ionization potential of hydrogen is nearly 1 Rydberg. See the discussion in Part 2 of this document for an exact definition and how to convert the Rydberg to other units.) A physically-motivated continuum spanning the full energy range should be specified if possible. The continuum can be specified as a fundamental form (such as blackbody emission, optically thin bremsstrahlung emission, or a power law with optional exponential cutoff), interpolated from tables of points, or as the radiation field transmitted through a cloud, as predicted by previous calculations. Additionally, a set of built-in continua (for instance, emergent continua from many model atmospheres, the observed Crab Nebula continuum, or several typical AGN continua) can be specified as look-up tables.

1.4.1.2. Continuum intensity and luminosity cases

The intensity of the external continuum striking the cloud must be specified. This can be given either as the flux striking a unit surface area of cloud or as luminosity radiated by the central object into 4π sr. There are many ways to set these.

The code must be able to derive the flux of photons (cm^{-2} s^{-1}) striking the illuminated face of the cloud. If the continuum is specified as a flux, the light striking a unit area of cloud, then the inner radius of the cloud does not need to be specified. If the inner radius is not specified then a plane parallel geometry will be assumed. A plane parallel geometry is simulated as a sphere with an inner radius of 10^{30} cm. The predicted emission-line spectrum will be given as intensities (energy radiated per unit surface area of cloud). If the luminosity of the central source is given, the light radiated into 4π sr, then the inner radius of the cloud *must* be specified and emission-line luminosities will be predicted.

Finally, beware that the word *intensity* used here does not have the precise definition found in radiative transfer theory. In the standard literature both the specific and mean intensities *I* and *J* are defined per unit solid angle. In the following the word "intensity" will be used to indicate the total energy arriving from or emitted into 4π sr. In this case the quantity is closest to $4\pi J$. I try to specify units whenever this distinction is important.

1.4.1.3. Combining several continua

Up to 100 continua of any form can be included as part of the total continuum. There must be exactly the same number of shape and luminosity specifications. The code will stop if there are not.

1.4.2. Chemical Composition

The program considers the lightest 30 elements in detail. Grains are not part of the default composition but can be included. All stages of ionization are treated, and all published charge exchange, radiative recombination, and dielectronic recombination processes are included as recombination mechanisms. Photoionization from valence and inner shells and many excited states, as well as collisional ionization by both thermal and supra-thermal electrons and charge transfer, are included as ionization mechanisms. The chemistry includes many molecules and will go to the fully molecular limit (H in H_2 and C or O in CO). Although the default composition is solar, several other standard mixtures can easily be specified, and an arbitrary composition can be entered.

1.4.3. Geometry

The geometry is always 1D spherical, but can be made effectively plane parallel by making the inner radius much larger than the thickness of the cloud. The default is for the gas to have constant density and to fully fill its volume, but other pressure laws and models with only part of the volume filled can be computed as well.

Cloudy normally assumes an open geometry, or one in which the gas has a very small covering factor (these terms are defined in Section 2 beginning on page 6 below, and in section 5.9 of AGN3). This can be changed with the **`sphere`** command (page 75 below) which sets the covering factor (defined on page 8 below) to a large enough value for continuous radiation escaping the cloud in the direction towards the central object to always interact with gas on the other side. This is a closed geometry. Line photons which cross the central hole interact with line-absorbing gas on the far side if **`sphere static`** is set but do not interact (because of a Doppler shift due to expansion) if **`sphere expanding`** is set. This case is the default when **`sphere`** is specified.

1.4.4. Velocity Structure

Normally, Cloudy assumes that only thermal motions broaden spectral lines and that there is no internal velocity structure. These assumptions can be changed. A component of microturbulence can be added with the **`turbulence`** command (page 100 below). A flow can be computed with the **`wind`** command (page 115 below).

1.5. What is computed and printed

Cloudy is driven by a set of command lines. These normally reside in a small input file which the code reads. The code creates an output file as the model is computed. The commands are four-letter keywords (either upper or lower case) followed by free-format numbers that may be mixed with letters. When Cloudy is executed as a stand-alone program standard input (*stdin*) is read for input and standard output (*stdout*) is used for output.

As an example, create a small file (say, called **`simple.in`**) containing the following lines:

```
title example input
hden 5 // log of hydrogen density, cm^-3
blackbody 50,000 // continuum shape is a 50,000K blackbody
ionization parameter –2  // intensity of blackbody is set with ionization parameter
```

Suppose that the code has been compiled to create the executable *cloudy.exe*. Then, the model described by the parameters in this input file could be computed by typing the following at the command prompt:

```
cloudy.exe < simple.in > simple.out
```

The output will be in the file *simple.out*.

It is also possible for a larger program to drive Cloudy directly by treating it as a subroutine. There are examples of doing this in Part 3 of this document and in the download you obtain from the web site.

The program begins by echoing the input commands, except for comment lines beginning with a #, %, `//`, or c_ (a space after the leading c). Comments are ignored. The input stream ends with either a blank line or the end-of-file. Some properties of the incident radiation field, such as luminosity and number of photons in certain frequency ranges, are then printed.

Cloudy works by dividing a nebula into a set of thin concentric shells, referred to as zones. The zones are chosen to have thicknesses that are small enough for the physical conditions across them to be nearly constant. Adaptive logic continuously adjusts the physical thicknesses of these shells to ensure this. Typically ~100 to 200 zones are computed in an optically thick model of an H II region. The physical conditions in the first and last zones are always printed and intermediate zones may be printed if needed (this is governed by the **`print every`** command described on page 133 below). The output for each zone begins with a line giving the zone number, its electron temperature, the distance from the center of the spherical nebula to the center of the zone, and some other properties of the solution. The next line gives the relative contributions of various emission lines to the radiation pressure, if this amounts to more than 5% of the gas pressure. The remaining lines give the relative populations of ionization stages of the other elements. Many details about the conditions within the zone are intermixed with these relative populations.

After the zone calculations are complete and the model is finished the code will explain why the calculation stopped. It is very important to confirm that the calculation stopped for the intended reason. Some warnings, cautions, or notes about the calculation may also be printed. The code is designed to be autonomous and self aware. This self checking will ensure that its range of validity is not exceeded. It will complain if it goes outside its range of validity, if it feels that some parameter has been incorrectly set, or if something surprising has happened during the calculation. This is an essential core feature of the code since it is now often used to generate grids of thousands of models, making it impossible to validate individual models by hand.

The final print out begins with a recapitulation of the entered commands, followed by the predicted emission-line spectrum. The first two columns of the emission-line spectrum give an identifying label and wavelength for each spectral line. The third column is the log of the luminosity [erg s^{-1}] or intensity [erg cm^{-2} s^{-1}] of the emission line, and the last column gives its intensity relative to the reference line. The reference line is Hβ by default and other emission lines can be chosen with the **`normalize`** command described on page 128 below. The third column will be either the luminosity or intensity. The luminosity (energy radiated by a shell of gas covering Ω sr of the central object) is predicted if the continuum is specified as a luminosity. The line intensity $4\pi J$ (the energy emitted per square centimeter of the gas slab) is predicted if the continuum is specified as an intensity. If the geometry is spherical but the continuum is specified as an intensity then the line intensities will be expressed per unit area at the inner radius. Only the strongest emission lines are printed; the relative intensity of the weakest line to print is adjusted with the **`print faint`** command (page 135 below).

The last pages of the output gives some averages of the ionization fractions over the slab, the optical depths in various lines and continua, the intensity of the continuum emerging from the cloud, and other properties of the nebula.

There is a vast amount of information that is computed but not given in the standard output file. Special output files are created with the **`punch`** commands described starting on page 138 below.

1.6. Acknowledgments

Part 3 of this document goes into acknowledgements in detail. The development of Cloudy has been assisted by many people over many years. It would not have been possible without twenty-nine years of continuous support by The National Science Foundation. This began with AST 80-2522, and has continued with grants 83-05094, 85-12414, 87-19607, 90-19692, 93-19034, 96-17083, 00-71180, 03-07720, and most recently AST 06-07028. The support of NASA through its ATP and LTSA programs have been vital. A generous allotment of computer time and support from the University of Kentucky Center for Computational Sciences is also gratefully acknowledged.

2. DEFINITIONS

2.1. Overview

This section defines many of the quantities used by Cloudy. I try to follow standard notation, such as that used by Mihalas (1978) or AGN3. Part 2 of this document goes into many of these quantities in greater detail.

This document has the following typographic conventions; *filename*, *variable*, **`command`**, and ***routine***.

2.2. Continua

Figure 1 shows several of the continua computed in the calculation.

2.2.1. Incident continuum

The *incident continuum* is the external continuum emitted by the central object and strikes the illuminated face of the cloud. It is specified in the commands that set up the calculation. Often the incident continuum is the only energy source for the cloud. As the incident continuum is transmitted through the cloud it is diminished by extinction.

2.2.2. Diffuse continuum

The *diffuse continuum* (often referred to as the diffuse radiation field or diffuse fields) is the radiation field emitted by gas and grains within the nebula. Examples include the Lyman, Balmer, or two-photon continua emitted by hydrogen. These fields are very nearly isotropic and can be significant sources of ionizing radiation under some circumstances.

The main difference between the calculation of a stellar atmosphere and a photoionized nebula is in the treatment of the diffuse fields. The gas albedo, which

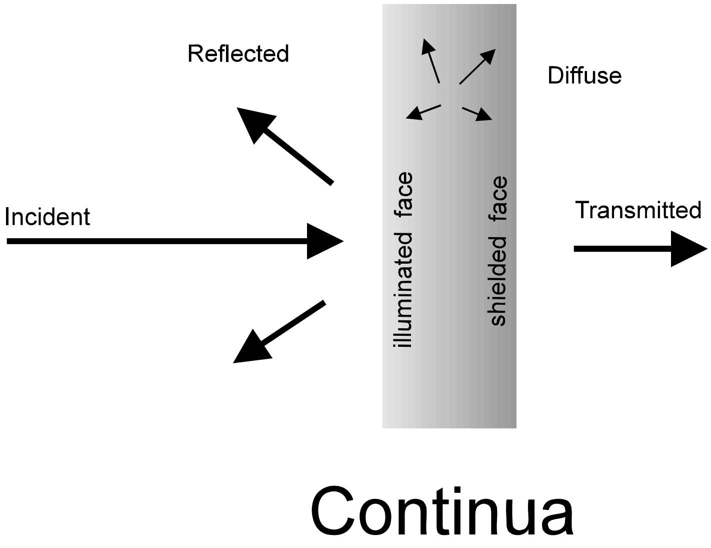


Figure 1 This figure illustrates several of the continua that enter in the calculations.

gives the relative probability of a photon being scattered versus being absorbed, is generally small in a nebula. As a result, the diffuse fields must be far weaker than the attenuated incident continuum, since the second is usually the cloud's only real energy source. The radiation field is usually dominated by the incident continuum. By contrast in a stellar atmosphere the nearly isotropic diffuse field usually dominates the local intensity. As a result the diffuse fields can be treated by lower order approximations in a nebula than in a stellar atmosphere.

2.2.3. Transmitted continuum

The *transmitted continuum* is the net continuum emergent from the shielded face of the cloud. It includes both the attenuated incident continuum and the transferred diffuse continuum.

2.2.4. Reflected continuum

The *reflected continuum* is the continuum emitted from the illuminated face of the cloud back into the direction towards (i.e., within 2π sr of) the source of the incident continuum. The reflected continuum is the result of both backscattered incident radiation and diffuse emission emitted from the cloud towards the source of ionizing radiation. This continuum is only computed for an *open geometry* (defined on page 9 below).

Figure 2 shows a plot of the incident and reflected continua for the Compton reflector in an AGN. This is a large column-density cloud, $10^{23.75}$ cm^{-2}, illuminated by

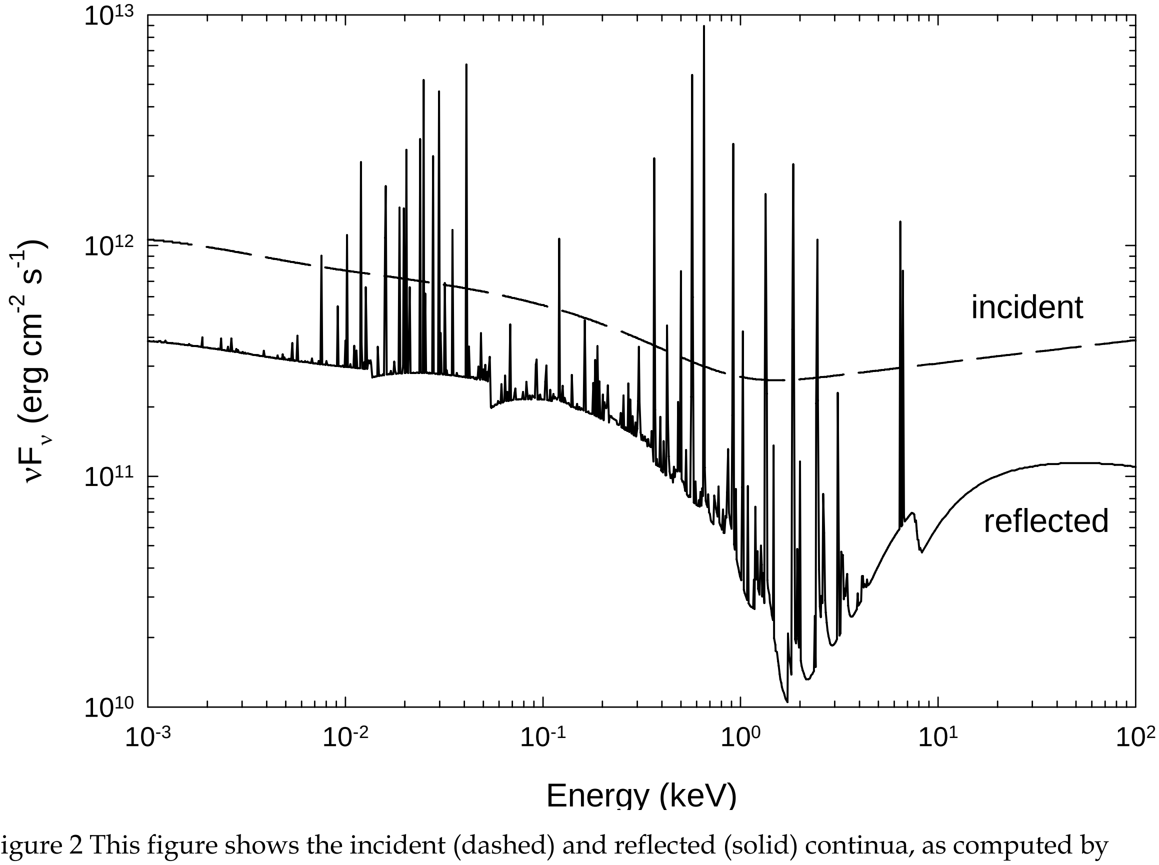


Figure 2 This figure shows the incident (dashed) and reflected (solid) continua, as computed by agn_blr_albedo.in in the test suite.

a $f_\nu \propto \nu^{-1}$ power law. The incident continuum is shown as a dashed line and the reflected continuum (obtained from the **`punch continuum`** command described on page 143 below). The Compton reflector's peak at X-ray energies is clearly shown.

2.3. Geometry

The geometry is always spherical, but can be changed to effectively plane parallel by making the inner radius much larger than the thickness of the cloud. In addition, it is possible to make the geometry nearly cylindrical, and a wind can be computed. The summary at the end of the calculation will say whether the geometry was plane parallel (the ratio of the thickness to the inner radius, $\Delta r/r_o < 0.1$), a thick shell ($\Delta r/r_o < 3$), or spherical ($\Delta r/r_o \geq 3$).

2.3.1. *Illuminated and shielded faces of the cloud*

The side of the cloud facing the source of ionizing radiation is the *illuminated face* of the cloud. The opposite side, in shadow, is referred to as the *shielded face* of the cloud. The illuminated face is generally hotter and more highly ionized than the shielded face.

2.3.2. *Depth and radius*

Figure 3 shows two possible geometries and some terms used to describe them. The *radius* is the distance from the center of symmetry, usually the center of the central object, to a given point. The *depth* is the distance between the illuminated face of the cloud and a point within the cloud. The *inner radius* is referred to as r_o, the *depth* is Δr, and the *current radius* is r. The depth or radius for a zone is the distance to the center of the zone.

2.3.3. *Covering factor*

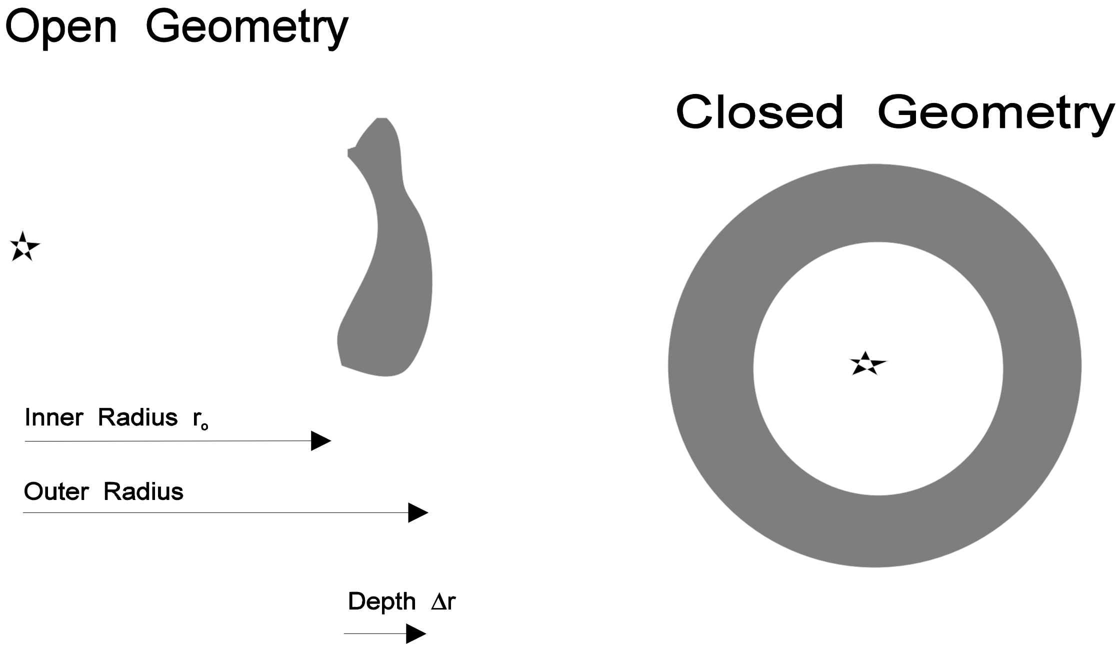


Figure 3 This figure shows the two limiting cases that can be assumed. The star is the source of ionizing radiation and the shaded area represents the cloud. An open geometry is the default, and a closed geometry will be computed if the **`sphere`** command is entered.

The *covering factor* is the fraction of 4π sr covered by gas, as viewed from the central source of ionizing radiation. It is normally written as $\Omega/4\pi$ (AGN3 Section 5.9), has the limits $0 \le \Omega/4\pi \le 1$, and is the fraction of the radiation field emitted by the central object that actually strikes nebular gas. *Line luminosities* give the total energy emitted by a shell covering Ω sr while line *intensities* give the energy emitted per unit area of cloud. Line luminosities scale nearly linearly with increasing covering factor, while line intensities are only weakly dependent on it. A section of Part 2 goes over the two covering factors that actually enter into the calculations.

2.3.4. Filling factor

The *filling factor f*(*r*) accounts for clumping of emission-line gas. When a filling factor is set the hydrogen density is the density within regions containing gas, while surrounding regions are assumed to be a vacuum. The specific effects of a filling factor are described by Osterbrock and Flather (1959), AGN3 section 5.9, and page 78 below.

2.3.5. Hydrogen density

The *hydrogen density n*(H) is the total hydrogen density given by

$$n(\mathrm{H}) = n\left(\mathrm{H}^0\right) + n\left(\mathrm{H}^+\right) + 2n\left(\mathrm{H}_2\right) + \sum_{other} n\left(\mathrm{H}_{other}\right) \ [\mathrm{cm}^{-3}] \qquad (1)$$

where $n(\mathrm{H}_{other})$ represents H in all other hydrogen-bearing molecules.

2.3.6. Column densities

The *hydrogen column density N*(H) is given by

$$N(\mathrm{H}) = \int n(\mathrm{H}) f(r)\, dr \ \ [\mathrm{cm}^{-2}] \qquad (2)$$

where *f*(*r*) is the filling factor. I try to consistently use lower case *n* for a volume density (cm^{-3}) and an upper case *N* for a column density (cm^{-2}).

2.3.7. Open vs. closed geometry

Two limiting cases, referred to as *open* and *closed*, can be identified for the geometry and its influence upon the calculations. Figure 3 shows examples of both. The covering factor determines which is the best approximation. The choice mainly affects the transfer of the diffuse fields and has only second-order effects on predicted quantities.

Open geometry. An *open* geometry is one in which the covering factor of the gas is small. All radiation that escapes from the illuminated face of the cloud, towards the source of continuous radiation, then escapes from the system without further interaction with gas. This is thought to be the case in, for example, the broad-line region of active nuclei or a blister H II region. In this case Lβ and higher hydrogen Lyman lines and ionizing radiation produced by recombinations can escape from the nebula. This geometry is the default and will be assumed if the **`sphere`** command is not specified.

Closed geometry. Emission-line gas covers ~4π sr as seen by the central object in a *closed* geometry. If the central object is small relative to the nebula then all diffuse fields which escape from the illuminated face of the cloud in the direction towards the central object will go on to strike the far side of the nebula. This geometry is implicitly assumed in most calculations of planetary nebulae and H II regions. This geometry will be assumed if the **`sphere`** command is entered (page 80 below).

Static vs. expanding. The **`sphere`** command has two optional arguments, **`static`** and **`expanding`**. This determines how emission-line photons which cross the central hole and strike the far side of the shell interact with the gas. The **`static`** option says to assume that the shell is stationary so that all lines interact across the nebula. In this case hydrogen Lyman line interaction should ensure that Case B is reached (AGN3 Section 4.2). If the nebula is expanding then the continuum photons that cross the central hole will interact with gas on the far side but the expansion velocity of the shell ensures that diffuse line photons do not. In this case the **`expanding`** option should be set. This second case is the default when **`sphere`** is specified with no options.

Don't panic! These geometrical considerations (open vs closed, static vs expanding) make only second-order differences in the predicted emission-line spectrum, generally at the ≈10% level, largely because of the different treatments of the radiative transfer of the diffuse fields. If you are concerned about which geometry to use, try both, and compare the results. The differences are usually small.

2.3.8. Matter-bounded and radiation-bounded geometries

Two limiting cases for the hydrogen-ionization structure of a cloud exist.

Matter-bounded geometry. The nebula is said to be matter bounded if the outer limit to the H^+ region is marked by the outer edge of the cloud. In this case the cloud is ionized throughout and is optically thin to the incident continuum. In a matter-bounded cloud the intensity or luminosity of an optically thin recombination line is set by the product of volume and density (called the emission measure n^2V , AGN3, Section 8.1) and is not directly related to the luminosity of the ionizing continuum.

Radiation-bounded geometry. The nebula is said to be radiation bounded if the outer limit to the H^+ region is defined by a hydrogen ionization front so both warm ionized and cold neutral regions exist. The H^+ region is optically thick to the hydrogen-ionizing continuum and has absorbed nearly all of it. In this case the intensity or luminosity of a recombination line is set by the luminosity of the ionizing continuum with relatively little dependence on cloud properties.

2.4. Intensity & luminosity cases

Cloudy must be able to deduce the surface flux of photons [cm^{-2} s^{-1}] at the illuminated face of the cloud. There are two ways to do this, referred to as the intensity and luminosity cases. The units of many of the predicted quantities will depend on which case is specified.

If the incident continuum is specified as either a “luminosity”, continuum radiated by the central object into 4π sr, then it is also necessary to specify an inner or starting radius and the emission lines will also be predicted as luminosities.

It is not necessary to specify a starting radius in the intensity case, although it is possible to do so. Line intensities (energy emitted per unit area of cloud, $4\pi J$) will be predicted if the starting radius is not given. A default starting radius of 10^{30} cm will be assumed if one is not specified. This should result in a plane-parallel geometry.

The incident continuum can be specified as an "intensity", the continuum incident onto a unit area of cloud, with units cm^{-2} s^{-1}, or a "luminosity", the continuum radiated by the central object into 4π sr, with units s^{-1}. Each of the following commands is characterized as either an intensity or luminosity command. The word "intensity" appears in quotes since it is not the *I* or *J* defined in radiative transfer texts, but rather the photon or energy equivalent of $4\pi J$.

2.4.1. Luminosity commands

If the continuum luminosity is set then the inner radius of the cloud *does* need to be specified, and emission-line luminosities are predicted. A covering factor will linearly change the luminosity of the entire spectrum, but will have only second order effects on relative intensities.

2.4.2. Intensity commands

If the continuum "intensity" is set then a starting radius *does not* need to be specified. If the starting radius is not specified then an inner radius of 10^{30} cm is assumed. A plane-parallel geometry usually results. The predicted emission-line spectrum is then given in intensity units. A starting radius may be specified and, if it is, then the resulting geometry may be spherical, plane parallel, or a thick shell, depending on the ratio of the outer to inner radii. Both absolute and relative intensities of lines have only second-order dependencies on the covering factor.

2.4.3. The units of the predicted emission lines

The units of the predicted emission-line spectrum are determined by the units of the continuum. If the incident continuum is specified as a luminosity then the spectrum will be given as the luminosity radiated by a shell covering Ω sr of the central object (L_{line}, erg s^{-1}). Here Ω is the angular coverage of the nebula so that $\Omega / 4\pi$ (with a default value of unity) is the covering factor (AGN3, Section 5.9, and page 77 below). If the continuum is specified as an intensity then the spectrum will be the energy radiated by a unit area of cloud into 4π sr ($4\pi J_{line}$, erg cm^{-2} s^{-1}).

3. INTRODUCTION TO COMMANDS

3.1. Overview

This section introduces the commands that drive Cloudy. The following chapters group the commands together by purpose. Individual commands are discussed after examples of their use. This section begins by outlining conditions that are assumed by default and then goes on to discuss the various classes of commands (i.e., those that set the continuum shape, luminosity, or the geometry).

3.2. Command parsing routines

I try very hard to keep this document parallel with the code. In case of any confusion, please consult the original source. The commands are parsed by the series of routines that have names beginning with "*parse*". The list of routines can be seen by listing the files *parse*.cpp*. The second half of the name indicates the command that is parsed by that routine.

3.3. Default conditions

Cloudy is designed to be easy to use, so that a minimum number of commands are

Table 1
Default Conditions

Quantity	Value	Command	page
Default inner radius	10^{30} cm	radius	79
Default outer radius	10^{31} cm	radius	79
Highest allowed temperature	10^{10} K		
Stop calculation when *T* falls below this value	4000 K	stop temperature	126
Relative error in heating-cooling balance	0.005	set temperature convergence	219
Relative error in electron density	0.01	set eden convergence	219
Relative intensity of faintest line to print	10^{-3}	print line faint	135
Low-energy limit to continuum	1.001×10^{-8} Ryd		
High-energy limit to continuum	7.354×10^{6} Ryd		
Limiting number of zones	1400	set nend	214
Total hydrogen column density	10^{30} cm^{-2}	stop column density	121
H^+ column density	10^{30} cm^{-2}	stop column density	121
H^0 column density	10^{30} cm^{-2}	stop column density	121
Grains?	No grains	grains	58
Line to continuum contrast	1000 km s^{-1}	set PunchLWidth	216
Background cosmic rays	No	cosmic rays	104
Cosmic background	No	background	30

needed to drive it. The general philosophy is for a reasonable set of initial conditions to be assumed by default. These default conditions are summarized in Table 1, which also lists the commands that change each assumption.

The code is also designed to check that its assumptions are not violated. It should complain if problems occur, if its limits are exceeded, or if the input parameters are unphysical. It may print a series of warnings, cautions, or notes if some limit was exceeded or physical assumption violated.

3.4. Command format

Input and Output. When executed as a stand-alone program Cloudy reads *stdin* for input and produces output on *stdout*. From a command prompt, this would be done as **`cloudy.exe < input > output`**. The code is also designed to be used as a subroutine of other, much larger, programs, often to generate large grids of simulations. In this case the input stream is entered using the subroutine calls described in a section of Part 3 of this document. In either case, this input stream must contain all the commands needed to drive the program. The command format is the same whether used as a stand-alone program or as a subroutine.

Command-line format. All commands are entered lines that start with a left-aligned four-character key word in columns 1 to 4. This keyword specifies the purpose of the command and is usually followed by one or more numbers or keywords. The keywords can be either lower or upper case. In the following examples the individual command keywords are shown extending beyond column 4. These extra characters are usually ignored.

The end of each command line is marked[2] by the end-of-line, a semi-colon ";", a pair of forward slashes "//", a sharp sign "#", or a percentage sign "%".

The command lines can be in any order and each can be up to 200 characters long[3]. The input stream ends with either a blank line or the end-of-file.

Units. Most commands use cgs units. In a few cases common astronomical nomenclature can be entered (i.e., the luminosity can be specified as erg s^{-1}, in solar units, or even magnitudes). This syntax varies from command to command so it is important that the units be checked carefully.

Number of commands. Up to 4000 separate commands may be entered.

Output as input. Cloudy can also read its own output as an input stream. As described in the section "Output" in Part 3 of this document, the code echoes the input command lines as a header before the calculation begins. These lines are centered on the page and surrounded by asterisks.

[2] Before version 92 a colon (":") could also mark an end of line. This character is needed to specify a path in the Windows environment and is no longer an end-of-line indicator.

[3] This limit is set by the length of the variable **`INPUT_LINE_LENGTH`** which occurs in a header file. Increase this variable and recompile the entire code if longer lines are needed.

Sometimes a particular model will need to be recomputed. You can do this by making a copy of the printed command lines and using this copy as an input file. The input parser will handle removal of the leading spaces and asterisk. This is mainly a debugging aid.

3.4.1. Syntax used in this document

Sections describing each of the commands are introduced by examples of their use.

Square brackets indicate optional parameters. Optional parameters are shown surrounded by square brackets ("[" and "]"). The examples shown below use the format given in this document.

```
// following needs flux density, but frequency is optional
f(nu) = -12.456 [at .1824 Ryd]
//
// the luminosity command has several optional keywords
luminosity 38.3 [solar, range, linear]
//
// the phi(h) command has the range option
phi(h) = 12.867 [range ...]
```

These square brackets indicate only that the parameters are optional. The brackets should not be placed on the command line. They will be totally ignored if they occur. The above exampe would actually be entered as follows:

```
// following needs flux density, but frequency is optional
f(nu) = -12.456 at .1824 Ryd
//
// the luminosity command has several optional keywords
luminosity 38.3 solar, range, linear
//
// the phi(h) command has the range option
phi(h) = 12.867 range ...
```

Underscores indicate a space. Most commands and keywords require four character matches to be recognized. In some cases the leading or trailing character is a space, which is indicated by an underscore ("_"; an example is the keyword **_LTE**). Other examples are shown below. The underscore must not be typed, only the space character. Only one space is needed between words.

The following is an example with the commands written as they are shown in this document:

```
// blackbody with T=50,000, in strict TE
blackbody 50,000 _lte
//
// use ISM radiation field
table _ism
```

The following is how the commands should actually be entered:

```
// blackbody with T=50,000, in strict TE
blackbody 50,000 lte
//
// use ISM radiation field
table ism
```

The space must occur where the underscore is written.

3.4.2. and, because nobody ever reads this document ….

The examples of commands show the square brackets and underscores for optional parameters and required spaces. Many people put these characters into the input stream because they don't read documentation. As a service to the user, the command-line parser will usually replace any square brackets or underscores with the space character when the command lines are initially read. The exception is any part of a string that is surrounded by double quotes. The string between double quotes is likely to be a file name and an underscore can occur in such a name.

3.4.3. The continue option

It may not be possible to enter all the required values on a single line for the **interpolate** and **abundances** commands. In these two cases the original command line can be continued on following lines with a series of lines beginning with the keyword **continue**. The format on a **continue** line is unchanged. There is no limit to the number of **continue** lines that can be included other than the limit of a total of 4000 input lines. The following is an example with the abundances command

```
abundances he =-1 li=-9 be=-11 b=-9 c=-4.3 n=-5 o=-2.3
continue f=-7 ne =-1.2 na =-3 mg =-8
continue al =-8 si =-8 p=-6 s=-8 cl=-9 ar =-8 k=-6
continue  ca =-8 sc=-9 ti=-7 v=-8 cr=-6.3 mn=-6 fe =-8
continue co =-9 ni =-8cu=-7 zn=-7
```

3.4.4. Numerical input

Numerical parameters are entered on the command line as free-format numbers. Exponential notation can be used[4]. Commas can be freely embedded in input numbers and they are completely ignored. Numbers may be preceded or followed by characters to increase readability. The strings "T=1,000,000K", "1000000", and "T=1E6" are equivalent. A period or full stop (".") by itself is interpreted as a character, not numeral or number.

Default values are often available. As an example, the **power law** command has three parameters, the last two being optional. The following are all acceptable (but not equivalent) forms of the command;

```
power law, slope-1.4, cutoffs at 9 Ryd and 0.01 Ryd
powe -1.0 5
power law, slope=-1.4 .
```

The last version uses the default cutoffs, i.e., none. If optional parameters are omitted they must be omitted from right to left; numbers must appear in the expected order.

Note that implicit negative signs (for instance, for the slope of the power law) *do not* occur in any of the following commands.

[4] Exponential notation could not be used in versions 07 and before.

Table 2
Interpretation of Numerical Input

Typed Quantity	Interpreted as	Why
1,000	1000	Commas are removed before parsing
1e2	100	Exponentional notation is OK
1e2,1e4	two numbers, 1e21 4	"," is removed
1.2.3	two numbers 1.2 0.3	1.2 is parsed, then .3
100,3.141516	1 number 1003.141516	Comma is removed
.3 3.	0.3 and 3.0	

Table 2 lists how various typed inputs will be interpreted. The first column gives the typed quantity, the second its interpretation, and the third an explanation.

3.4.5. Comments

Comments may be entered among the input data in several ways. Comments can be entered at the end of a command line after a semi-colon (";"), double slash ("//"), a sharp sign ("#"), or a percentage sign ("%"). Anything on a line after one of these characters is completely ignored. This can be used to document parameters on a line. Any line beginning with a #, %, //, or a * is totally ignored; it is not even printed. A line beginning with c_ is ignored, but printed (note that there is a space after the c). There is also a **title** command, to enter a title for the simulation, as described on page 173 below.

3.4.6. Hidden commands

A command will be parsed and used by the code but not printed in the output if the keyword **hide** occurs somewhere on the command line. This provides a way to not print extensive sets of commands, like the **continue** option on the **continuum** command, or the **print off** command in an initialization file.

3.4.7. Log vs linear quantities

I have tried to keep the input quantities as logical as possible. Most quantities are entered as the log of the number but some are linear. The following outlines some systematics of how these are entered.

Temperature. Cloudy will interpret a temperature as a log if the number is less than or equal to 10 and the linear temperature if it is greater than 10. Many commands have the optional keyword **linear** to force numbers below 10 to be interpreted as the linear temperature rather than the log.

Other parameters. The pattern for other quantities is not as clear as for the case of temperature. Often quantities are interpreted as logs if negative, but may be linear or logs if positive (depending on the command). Many commands have the keywords **_log** and **linear** to force one or the other interpretation to be used.

3.4.8. An example

Specific commands to set boundary conditions for a simulation are discussed in the following sections. As a minimum, the hydrogen density, continuum shape, continuum luminosity or intensity, and possibly the starting radius, must be specified to compute a model. As an example, a simple model of a planetary nebula could be computed by entering the following input stream.

```
title - this is the input stream for a planetary nebula
//
// set the temperature of the central star
blackbody, temperature = 100,000K
//
// set the total luminosity of the central star
luminosity total 38 // log(Ltot)- ergs/s
radius 17   // log of starting radius in cm
hden 4      // log of hydrogen density - cm^-3
sphere // this is a sphere with large covering factor
```

3.5. Filenames

It is sometimes necessary to read or write external files whose names are specified on a command line. File names are entered inside pairs of double quotes, as in "name.txt".

The command parser first checks whether a quote occurs anywhere on the command line. If one does occur then the parser will search for a second pair of quotes and use whatever text lies between as a filename. The code will stop with an error condition if the second of the pair of quotes is not found or if the file cannot be opened for reading or writing.

3.6. The `init` command

This is a special command that tells the code to read a set of commands stored in an ancillary file. This allows frequently used commands to be stored in a single file. The **`init`** command will automatically find initialization files that are located in the code's data directory, allowing them to be easily accessed from other directories. The code will first search for the file in the local directory and then on the path. The **`init`** command is fully described in the section beginning on page 200 below.

Any filename can be specified within a pair of double quotes, as in "ism.ini". The default name for the initialization file is *cloudy.ini*. There is no limit to the number of commands that can be in this initialization file other than the total limit of 4000 command lines that is intrinsic to the code.

This provides an easy way to change the default behavior of the code. For instance, many of the elements now included in Cloudy have negligible abundances and the code will run a bit faster if they are turned off with the **`element off`** command (page 55 below). Also, only about half of these elements were included before version 86 of the code. I normally keep a file called *c84.ini* in the Cloudy data directory which will make the current version of the code behave more like version 84. My *c84.ini* file contains the following commands:

```
print off hide
elements read
helium
carbon
```

```
nitrogen
oxygen
neon
sodium
magnesium
aluminium
silicon
sulphur
argon
calcium
iron
nickel
end  of elements
element Lithium off
element Beryllium off
element Boron  off
element Fluorine  off
element Phosphor off
element Chlorine off
element Potassium off
element Scandium  off
element Titanium off
element Vanadium off
element Chromium off
element Manganese off
element Cobalt off
element Copper off
element Zinc  off
print on
```

The current version of the code would only include those elements present in version 84 if the command

```
init "c84.ini"
```

were entered.

A series of _*.ini_ files are included in the data directory that comes with the Cloudy distribution. Do an “**ls *.ini**” within the data directory to list the available files. Comments at the start of the files describe their purpose.

3.7. Commands for experimental parts of the code

The code is in continuous development. When new gold versions are released at the start of a new year there will be new or experimental parts of the code that are still being developed or which have not been fully debugged. The newly-developed physics is not included in a calculation which uses the default conditions. The commands which exercise these new features are included in this document. Commands which exercise new physics are indicated two ways. First the ☠ symbol which starts this paragraph. Second the grey background. You are welcome to give these commands a try but should not expect robust results.

4. DEFINING THE CONTINUUM

4.1. Overview

The incident continuum should be defined between the low-energy limit to the code, 1.001×10^{-8} Ryd, and the high-energy limit of 7.354×10^{6} Ryd. The continuum shape and its intensity or luminosity are usually specified independently. There are many ways to do this.

4.2. The coarse and fine continua

The spectral resolution is defined as $E/\delta E$, where E is the photon energy and δE the resolution element. The number of energy bins needed to store the continuum is proportional to this resolution. The resolution is a major pace setter for the code since it must continuously reevaluate various integrals over the continuum.

The code uses multi-grid methods to compute interactions between the continuum and the many millions of spectral lines (Shaw et al. 2005). The coarse continuum is used to define the incident and diffuse continua and is output with various **`punch continuum`** commands. The resolution of the coarse continuum is defined in the file *continuum_mesh.ini* in the data directory. This file is designed to be changed by the user and can be changed to much higher resolution if need be. This is all described in the Chapter "The Continuum Mesh" in Part 3 of this document.

A second fine continuum has much higher spectral resolution and is far more expensive to evaluate. It is used to resolve overlapping spectral lines and define blocking coefficients for the coarse continuum. This permits the effects of line overlap and velocity shear to be treated automatically.

4.3. Defining a single continuum

Two quantities, the *shape* and *intensity*, specify a single continuum. The intensity can be either the surface flux of ionizing photons striking the illuminated face of the cloud or both the continuum luminosity and the cloud's inner radius. The shape and intensity are specified independently in most cases, although some commands specify both (the command specifying the cosmic microwave background is an example of the latter).

4.3.1. Continuum shape

The continuum shape can be set by interpolating on tables of points, read in from predictions of previous calculations, or by specifying fundamental forms such as blackbody, power law, or bremsstrahlung emission. Individual commands to specify the continuum shape are given in the chapter beginning on page 29 below.

4.3.2. Continuum intensity or luminosity

The intensity of the continuum at the illuminated face of the cloud can be specified as either an intensity (energy or photon flux per unit area) or by specifying *both* the luminosity *and* the inner radius (i.e., separation between the continuum source and the illuminated face) of the cloud. These are referred to as the intensity and luminosity cases respectively. Individual commands that are used to specify the continuum luminosity or intensity are given in the chapter beginning on page 22 below.

The following discussion will refer to luminosity commands to mean either luminosity or intensity commands.

4.4. Combining several continua

4.4.1. The sum of several continuum

It is possible to combine up to 100 continua.[5] Cloudy will stop if more than 100 continua are entered. This limit is set by the variable ***LIMSPC*** that occurs in one of the included header files.

When more than one continuum is entered the series of luminosity and shape commands must be in the same order (i.e., map one to one). There must always be exactly the same number of luminosity and shape specifications; Cloudy will stop if there are not.

As an example, the following would be a rough approximation of an accretion disk and boundary layer around a white dwarf:

```
// this is the black body associated with the boundary layer
black body, temperature =500,000K
luminosity (total) 37.3
// the following is a rising power law, a simple approximation to the disk
power law, slope = 1.333, cutoff = 0.6 Ryd
luminosity (total) 37.2
```

The 500,000 K blackbody is given a total luminosity of $10^{37.3}$ erg s^{-1}, while the power-law continuum is given a total luminosity of $10^{37.2}$ erg s^{-1}.

4.4.2. Keeping shape and intensity commands together

It is not absolutely necessary to keep the ordered pairs of shape and luminosity commands together but this is a good practice since some commands (those given in Table 3) specify *both* the continuum shape and intensity. Problems arise if one of the commands giving both shape and intensity is entered between another pair of shape and intensity commands. For instance, the following will produce unintended results:

```
black body, temp = 500,000K
CMB, z=2
luminosity (total) 37
```

because the **CMB** command enters both the shape and intensity of the cosmic microwave background. In this example it comes after the

Table 3
Commands specifying both shape *and* intensity

background
blackbody, energy density
blackbody, LTE
blackbody, luminosity
blackbody, radius
CMB
table Draine
table HM96, HM05
table ISM

[5] Restrictions on the number of tables that could be entered existed in Cloudy versions 73 and before, but have been lifted. Restrictions on which types of continua could be combined existed in Cloudy versions 67 and before, but have been lifted.

blackbody command specifies a shape, but before the **luminosity** command specifies the luminosity of the blackbody. As a result the intensity implicitly entered by the **CMB** command will apply to the hot blackbody continuum rather than the cosmic microwave background and the **luminosity** command will then incorrectly set the intensity of the cosmic background blackbody shape. This problem cannot occur if the shape and luminosity commands are always kept together as in the previous example. The code should produce a warning if shape and luminosity commands are mixed together with a command that enters both.

4.5. Check the continuum!

It is important to check that the continuum has been entered correctly. First set up the commands to do a simulation and include the **punch continuum** command as described on page 143 below. Do the simulation and examine the file produced by the **punch continuum** command. The first column gives the photon energy and the second gives incident continuum (as νJ_ν, erg cm^{-2} s^{-1}) at the illuminated face of the cloud. Plot this continuum and check that it is correct.

5. CONTINUUM LUMINOSITY

5.1. Overview

All commands setting the intensity or luminosity of the continuum are defined in this Chapter.

5.2. The range option

Many of the intensity/luminosity commands specify the number of photons or energy *in hydrogen-ionizing radiation* (1 Ryd $\le h\nu \le 7.354\times10^{6}$ Ryd). Other energy intervals can be specified with the **`range`** option, an optional keyword that can appear on most intensity / luminosity commands.

When the keyword **`range`** appears there are an additional two parameters, the low- and high-energy limits to the energy range in Rydbergs. These appear as the second and third numbers on the line (the first number giving the intensity or luminosity). The position of the keyword **`range`** on the command line does not matter but the order of the numbers on the line does matter. If either of the range parameters is zero then the low (1.001×10^{-8} Ryd) or high (7.354×10^{6} Ryd) energy limit of the continuum will be substituted for the zero value. If both energies are specified then the second number must be larger than the first, unless the second is zero, in which case it is the default high-energy limit of the code. If only one parameter appears then only the lower limit of the range will be changed and the high-energy limit will be left at its default of 7.354×10^{6} Ryd. If the first optional number is negative or the keyword **`_log`** appears then *both* of the extra numbers are interpreted as logs[6].

If **`range total`**, or simply **`total`**, appears with no parameters then the full energy range considered by the program, 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd, will be used. In this case the number is the total integrated intensity or luminosity.

The following shows examples of the range option for the **`luminosity`** command. By default the **`luminosity`** command has a single parameter, the log of the luminosity [erg s^{-1}] in hydrogen-ionizing radiation (1 Ryd $\le h\nu < 7.354\times10^{6}$ Ryd). The ";" symbol is used to terminate the line in one case.

```
// this will use the default range, only ionizing radiation
luminosity 38 ;the log of the luminosity in erg s^-1

// either will be the total luminosity
luminosity total 38
luminosity range total 33.4

// this will be the luminosity in visible light
luminosity 37.8 range .15 to .23 Ryd
```

[6] The command parser replaces a zero with one of the energy bounds of the code before it checks for the log option and converts the entered numbers into linear energy bounds. This poses a problem if an energy bound of 1 Ryd is used with the **`log`** option, since **`log range 0`** will be interpreted as a energy bound given by dex of the actual energy range. Don't use the **`log`** option and an energy bound of 1 Ryd together.

```
// the luminosity in radiation more energetic than 0.1 Ryd
luminosity 38.1 range -1

// this will be the luminosity in non-ionizing radiation
luminosity 39.8 range 0 1
```

5.3. absolute [visual, bolometric] magnitude -2.3

It is possible to specify the integrated or monochromatic luminosity in "magnitudes", a quaint unit of historical interest. One of the keywords **bolometric** or **visual** must also appear. The absolute bolometric magnitude M_{bol} is related to the total luminosity by (Allen 1976, page 197)

$$L_{total} = 3.826 \times 10^{33} \times 10^{(4.75 - M_{bol})/2.5} \text{ [erg s}^{-1}\text{]} . \qquad (3)$$

The absolute visual magnitude M_V is approximately related to the monochromatic luminosity per octave at 5550 Å by (Allen 1976, page 197)

$$\nu L_\nu\left(5500\text{Å}\right) \approx 2.44 \times 10^{35} \times 10^{-M_V/2.5} \text{ [erg s}^{-1}\text{]} . \qquad (4)$$

The conversion between monochromatic luminosity per octave νL_ν and absolute visual magnitude M_V is approximate, with typical errors of roughly a percent. This is because Cloudy assumes that the V filter has an isophotal wavelength of 5550Å and does not actually integrate over the incident continuum using a V-filter transmission function.

This is a luminosity command.

5.4. energy density 50,000K [linear]

This specifies the energy density [K] of the incident radiation field. The number is the equivalent energy-density temperature, defined as $T_u = (u/a)^{1/4}$ where u is the total energy density in all radiation [erg cm^{-3}] and a is the Stefan radiation-density constant. The number is interpreted as the temperature itself if it is greater than 10 and as the log of the number if it is less than or equal to 10. The optional keyword **linear** forces the number to always be interpreted as a linear temperature.

This is an intensity command.

5.5. f(nu) = -12.456 [at .1824 Ryd]

This specifies the monochromatic intensity at an arbitrary energy. The first number is the log of the monochromatic mean intensity at the illuminated face of the cloud, $4\pi J_\nu$ (with units erg s^{-1} Hz^{-1} cm^{-2}), where J_ν is the mean intensity of the incident continuum per unit solid angle.

The optional second number is the frequency in Rydbergs where $4\pi J_\nu$ is specified. The default is 1 Ryd. In the example above the continuum is specified at 0.1824 Ryd = 5000Å. The frequency can be any within the energy band considered by the code, presently 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd. If the energy is less than or equal to zero then it is interpreted as the log of the energy in Rydbergs, and as the linear energy itself if positive.

This is an intensity command.

5.6. intensity 8.3 [range, linear]

This specifies the integrated intensity, $4\pi J$, [erg cm^{-2} s^{-1}] at the illuminated face of the cloud

$$4\pi J = \int_{\nu_1}^{\nu_2} 4\pi J_\nu \, d\nu \quad [\text{erg s}^{-1}\ \text{cm}^{-2}] \, . \tag{5}$$

This is the per unit area equivalent of the **luminosity** command (see page 25 below). The number is the log of the intensity unless the optional keyword **linear** appears. Unlike the majority of the commands, the first five characters of the line must be entered.

The default range is over hydrogen-ionizing energies (1 Ryd $\le h\nu \le 7.354\times10^{6}$ Ryd). The **range** option can be used to adjust the values of ν_1 and ν_2.

Some of the interstellar medium and photo-dissociation region (PDR) literature specifies the incident continuum in units of the Habing (1968) field (see, for instance, Tielens and Hollenbach 1985a, 1985b). This radiation field has an integrated intensity of 1.6×10^{-3} erg s^{-1} cm^{-2} between the limits of 6 and 13.6 eV (Tielens and Hollenbach 1985a; Hollenbach, Takahashi & Tielens 1991). This integrated intensity is sometimes referred to as G_o. The continuum described by Tielens and Hollenbach, but with an intensity of 1 G_o, could be generated with the commands:

```
// a B star with an intensity roughly the Habing 1968 radiation field
blackbody 30,000K
intensity -2.8, range 0.44 to 1 Ryd
extinguish by 24, leakage = 0
```

This set of commands sets the shape of the Balmer continuum to that of a hot blackbody, sets the intensity to the Habing value, and then extinguishes all hydrogen-ionizing radiation, as is assumed in the PDR literature.

This is an intensity command.

5.7. ionization parameter = -1.984

The ionization parameter is the dimensionless ratio of hydrogen-ionizing photon to total-hydrogen densities. It is defined as

$$U \equiv \frac{Q(\mathrm{H})}{4\pi r_o^2\, n(\mathrm{H})c} \equiv \frac{\Phi(\mathrm{H})}{n(\mathrm{H})c} \tag{6}$$

(AGN3, equation 14.7, page 357). Here r_o is the separation [cm] between the center of the source of ionizing radiation and the illuminated face of the cloud, n(H) [cm^{-3}] is the total[7] hydrogen density (ionized, neutral, and molecular), c is the speed of light, Q(H) [s^{-1}] is the number of hydrogen-ionizing photons emitted by the central object, and Φ(H) [cm^{-2} s^{-1}] is the surface flux of ionizing photons. The number is interpreted

[7] Before version 65 of the code the electron density was used rather than the hydrogen density. Before version 75 n(H) was the atomic/ionic hydrogen density, and did not include molecules.

as the log of *U* unless the keyword **linear** appears. The ionization parameter is a useful quantity in plane-parallel, low-density, constant-density, models, because of homology relations between models with different photon and gas densities but the same ionization parameter (see Davidson 1977).

This is an intensity command.

5.8. L(nu) = 24.456 [at .1824 Ryd]

This sets the monochromatic luminosity L_ν [erg s^{-1} Hz^{-1}] of the central object. The first number is the log of the luminosity. The optional second number is the frequency in Rydbergs where L_ν is specified. The default is 1 Ryd. In the example above the continuum is specified at 0.1824 Ryd = 5000 Å. The frequency can be any within the energy band considered by the code, presently 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd. If the energy is less than or equal to zero then it is interpreted as the log of the energy in Rydbergs, and the linear energy itself if positive.

This is a luminosity command.

5.9. luminosity 38.3 [solar, range, linear]

The number is the log of the integrated luminosity[8] emitted by the central object into 4π sr,

$$L = 4\pi R_{star}^2 \int_{\nu_1}^{\nu_2} \pi F_\nu \, d\nu \;\; [\text{erg s}^{-1}]. \qquad (7)$$

The default range is over hydrogen-ionizing energies (1 Ryd ≤ $h\nu$ ≤ 7.354×10^{6} Ryd). The **range** option can be used to adjust the values of ν_1 and ν_2.

The number is interpreted as the log of the *total* luminosity relative to the luminosity of the sun if the optional keyword **solar** appears. It is the log of the total luminosity if the keyword **total** appears. If the **linear** keyword is also used then the quantity will be the luminosity itself and not the log. The **range** option cannot be used if the luminosity is the total luminosity or it is specified in solar units. It will be ignored if it appears.

The following are examples of the luminosity command.

```
// log of luminosity (erg/s) in ionizing radiation
luminosity 36

// roughly the Eddington limit for one solar mass
luminosity total 38

// both are a total luminosity 1000 times solar
luminosity solar 3
luminosity linear solar 1000

// this will be the luminosity in visible light
luminosity 37.8 range .15 to .23 Ryd
```

[8] Before version 83 of the code, the luminosity command was used to enter both luminosity and intensity. The code decided between the two by checking on the resulting ionization parameter. There are now separate intensity and luminosity commands.

This is a luminosity command.

5.10. nuF(nu) = 13.456 [at .1824 Ryd]

This command specifies the log of the monochromatic mean intensity per octave $4\pi \nu J_\nu$ [erg s^{-1} cm^{-2}] at the illuminated face of the cloud. Here J_ν is the mean intensity of the incident continuum.

The optional second number is the frequency in Rydbergs where $4\pi \nu J_\nu$ is specified. The default is 1 Ryd. In the example above the continuum is specified at 0.1824 Ryd = 5000Å. The frequency can be any within the energy band considered by the code, presently 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd. If the energy is less than or equal to zero it is interpreted as the log of the energy in Rydbergs. It is the linear energy if it is positive.

This is an intensity command.

5.11. nuL(nu) = 43.456 [at .1824 Ryd]

This command specifies the monochromatic luminosity per octave νL_ν [erg s^{-1}]. The first number is the log of the luminosity radiated by the central object into 4π sr. It can be expressed at an arbitrary photon energy but the default is 1 Ryd.

The optional second number is the frequency in Rydbergs where L_ν is specified. In the example above the continuum is specified at 0.1824 Ryd = 5000Å. The frequency can be any within the energy band considered by the code, presently 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd. If the energy is less than or equal to zero, it is interpreted as the log of the energy in Rydbergs, and the linear energy if positive.

This is a luminosity command.

5.12. phi(H) = 12.867 [range ...]

This command specifies the log of Φ(H), the surface flux of hydrogen-ionizing photons [cm^{-2} s^{-1}] striking the illuminated face of the cloud. It is defined as

$$\Phi(\mathrm{H}) \equiv \frac{Q(\mathrm{H})}{4\pi r_o^2} \equiv \frac{R_{star}^2}{r_o^2} \int_{\nu_1}^{\nu_2} \frac{\pi F_\nu}{h\nu} d\nu \ \ [\mathrm{s^{-1}\ cm^{-2}}] \tag{8}$$

and is proportional to the optical depth in excited lines, such as the Balmer lines (Ferland, Netzer, & Shields 1979; AGN3). The **range** option can be used to change the default energy range, given by the values of ν_1 and ν_2.

This is an intensity command.

5.13. Q(H) = 56.789 [range ...]

This is the log of the total number of ionizing photons emitted by the central object [s^{-1}]

$$Q(\mathrm{H}) = 4\pi R_{star}^2 \int_{\nu_1}^{\nu_2} \frac{\pi F_\nu}{h\nu} d\nu \quad . \tag{9}$$

The default energy range is 1 Ryd to 7.354×10^6 Ryd and the **range** option can be used to change the energy bounds ν_1 and ν_2. The photon flux (the number of photons per unit area of cloud surface) can be specified with the **phi(h**) command, described on page 26 above[9].

This is a luminosity command.

5.14. ratio -3.4 0.3645 Ryd to 147 Ryd [alphaox, _log]

This specifies the intensity of a second continuum source (referred to as the *current* continuum source) relative to the intensity of the *previous* continuum source. The ratio of the intensities $4\pi J_\nu$ (erg cm^{-2} s^{-1} Hz^{-1}) of the current to the previous continuum source is given by the first number on the command line. It is assumed to be the linear ratio unless it is less than or equal to zero, in which case it is interpreted as a log. If the keyword **_log** appears then the positive number is interpreted as the log of the ratio.

The second parameter is the energy in Rydbergs where the previous continuum source is evaluated and the optional third parameter is the energy where the current continuum is evaluated. If the second energy is not entered then the same energy is used for both. The following is an example of using the **ratio** command to simulate the continuum of a typical quasar.

```
blackbody 50,000        // the big blue bump
ionization parameter -2 // its ionization parameter
table power law         //an alpha =-1 power law
// now set intensity of power law relative to bump at 1 Ryd
ratio 0.001 at 1 Ryd;
```

This command was introduced to provide a mechanism to specify the optical to X-ray spectral index α_{ox}. This is defined here as in Zamorani et al. (1981), except for a difference in sign convention. Here α_{ox} is the spectral index which would describe the continuum between 2 keV (147 Ryd) and 2500Å (0.3645 Ryd) if the continuum could be described as a single power-law, that is,

$$\frac{f_\nu\left(2\ \text{keV}\right)}{f_\nu\left(2500\ \text{Å}\right)} = \left(\frac{\nu_{2\ \text{keV}}}{\nu_{2500\ \text{Å}}}\right)^{\alpha_{ox}} = 403.3^{\alpha_{ox}} \quad . \tag{10}$$

The definition of α_{ox} used here is slightly different from that of Zamorani et al. since implicit negative signs are *never* used by Cloudy. Typical AGN have α_{ox} ~ -1.4. If X-rays are not present then α_{ox} = 0.

The **ratio** command has an optional keyword, **alphaox**, which allows α_{ox} to be specified directly. If the keyword appears then only one parameter is read, the value of α_{ox}. A generic AGN continuum could be produced with the following,

[9] Before version 83 of the code the phi(H) and Q(H) commands were the same. The code decided which was specified by checking the order of magnitude of the resulting ionization parameter. These are now two different commands.

```
blackbody 50,000   // the big blue bump
ionization parameter -2
table power law    // an alpha =-1 power law
ratio alphaox -1.4 // set alpha_ox of the X-ray and UV continua
```

Note that α_{ox} may (or may not) depend on the luminosity of the quasar, as described by Avni and Tananbaum (1986). The solid line in their Figure 8 corresponds to

$$\alpha_{ox} = -1.32 - 0.088 \times \log\left(\frac{L_o}{10^{28}\ \mathrm{erg\,s^{-1}\,Hz^{-1}}}\right) \qquad (11)$$

where they define L_o as the monochromatic optical luminosity at 2500Å in the source rest frame, and assume $H_0 = 50$ and $q_0 = 0$. Other fits are given by Worral et al. (1987):

$$\alpha_{ox} = -1.11 - 0.111 \times \log\left(\frac{L_o}{10^{27}\ \mathrm{erg\,s^{-1}\,Hz^{-1}}}\right) \qquad (12)$$

and by Wilkes et al (1994):

$$\alpha_{ox} = -1.53 - 0.11 \times \log\left(\frac{L_o}{10^{30.5}\ \mathrm{erg\,s^{-1}\,Hz^{-1}}}\right) \ . \qquad (13)$$

However, LaFranca et al (1995) find no dependence of α_{ox} on luminosity. Avni, Worrall, and Morgan (1995) find a complicated luminosity dependence. Clearly this is an area of active research.

N.B. The net continuum may have a smaller than specified ratio of current to total continuum, since the command specifies the ratio of the current to the previous continuum, not the ratio of current to total continuum. The ionization parameter will be slightly larger than specified for the same reason.

In general, it is probably better to use the **AGN** command (described on page 29 below) rather than this command.

This is neither a luminosity nor intensity command — the units of the previous continuum carry over to this command.

5.15. xi –0.1

Tarter, Tucker, & Salpeter (1969) defined an ionization parameter ξ given by

$$\xi = \frac{L_{ion}}{n(\mathrm{H})r^2} = (4\pi)^2 \int_{1R}^{1000R} J_\nu \, d\nu \ / n(\mathrm{H}) \ [\mathrm{erg\ cm\ s^{-1}}] \qquad (14)$$

where n(H) is the hydrogen density at the illuminated face of the cloud and r is the source – cloud separation. L_{ion} is the luminosity between 1 and 10^3 Ryd. The number is the log of ξ. Only the first two characters on the line are checked to match **xi**, unlike the majority of commands where the first four characters on the line must match.

6. SPECTRAL ENERGY DISTRIBUTION SHAPE

6.1. Overview

The shape of the spectral energy distribution (SED) should be specified between the energies of 1.001×10^{-8} Ryd ($\lambda \approx 10$ m) and 100 MeV $\approx 7.354\times10^{6}$ Ryd. The low-energy region is important for Compton cooling, photoionization from excited states of the elements, free-free heating, H^- heating, and grain heating. The high-energy portion is important for Auger and secondary ionization, Compton heating, and pair production. Energies greater than 100 MeV are not generally important since the Klein - Nishina electron-scattering cross section is small. Cloudy will complain, but compute the model if possible, if the SED is not specified over the full energy range. An intensity of zero will be assumed for missing portions of the continuum.

The plasma frequency, given by

$$\nu_{pl} = \left(\frac{n_e q_e^2}{\pi\, m_e} \right)^{1/2} = 8.978\times10^{3}\, n_e^{1/2}\, s^{-1} = 2.729\times10^{-12}\, n_e^{1/2}\ \mathrm{Ryd}\,, \qquad (15)$$

will move into the energy range considered by the code if the electron density is higher than $\sim10^{7}$ cm^{-3}. The incident radiation field below the plasma frequency is totally reflected and does not enter the slab. The code will generate a comment if the plasma frequency occurs within the energy grid.

It is a good idea to plot the SED using the output of the **`punch continuum`** command (page 143 below).

Most incident radiation fields are assumed to strike the cloud as a single-directional beam. The beam is assumed to enter the slab normal to the surface, unless this is changed with the **`illumination angle`** command (see page 79 below). The **`background`**, **`CMB`**, **`table Drain`**, **`table HM96`**, **`table HM05`**, and **`table ISM`** commands all generate continua that are isotropic.

6.2. AGN T =150,000k, a(ox) = -1.4, a(uv)=-0.5 a(x)=-1

This produces a multi-component continuum similar to that observed in typical Active Galactic Nucleus (AGN). An example is shown in Figure 4. The “Big Bump” component, peaking at ≈1 Ryd, is a rising power law with a high-energy exponential cutoff. It is parameterized by the temperature of the bump, the first argument on the command line. It is interpreted as the log of the temperature if it is less than or equal to 10 and the linear temperature otherwise. The second parameter is the X-ray to UV ratio α_{ox} (see the discussion of $\alpha_{\rm ox}$ beginning on page 27 above). Note that there is no implicit negative sign in this exponent; typical AGN have $\alpha_{ox} \sim$ -1.4, (Zamorani et al. 1981). The third (optional) argument is the low-energy slope of the Big Bump continuum, with the default α_{uv} = -0.5 (Elvis et al. 1994; Francis 1993). The last argument is the slope of the X-ray component with the default α_x = -1. Optional parameters can be omitted from right to left.

The full continuum is the sum of two components, as in equation 16:

$$f_\nu = \nu^{\alpha_{uv}} \exp\left(-h\nu / kT_{BB}\right) \exp\left(-kT_{IR} / h\nu\right) + a\nu^{\alpha_x} \quad . \qquad (16)$$

The coefficient a is adjusted to produce the correct α_{ox} for the case where the Big Bump does not contribute to the emission at 2 keV. If the bump is very hot then it may contribute to the X-rays as well and the resulting continuum will have a more negative α_{ox} than specified. The X-ray power law is only added for energies greater than 0.1 Ryd to prevent it from extending into the infrared, where a power law of this slope would produce *very* strong free-free heating. The Big Bump component is assumed to have an infrared exponential cutoff at kT_{IR} = 0.01 Ryd.

The last term in equation 16 is not extrapolated below 1.36 eV or above 100 keV. Below 1.36 eV the last term is simply set to zero (the bump dominates for these energies). Above 100 keV the continuum is assumed to fall off as ν^{-2}.

The exponential cutoff in the low-energy end of the Big Bump will cause the incident continuum to have zero intensity at very long wavelengths. The code will complain since a zero incident continuum is unphysical, but the model will be computed. You can prevent the continuum from going to zero by including the cosmic background with the **`background`** command (described on page 30 below) or with the **`CMB`** command (described on page 33 below).

We used this command to generate the continuum used in a large atlas of BLR line intensities (Korista et al. 1997). The specific parameters needed to reproduce that continuum are **`AGN 6.00 -1.40 -0.50 -1.0`**. Only Kirk Korista can remember all these numbers, and the parameters were not explicitly given in the original paper in the format used by the code so the **`kirk`** option on the **`AGN`** command will generate that continuum. It is fairly similar to the Mathews & Ferland (1987) continuum but there is much greater flexibility in changing its details.

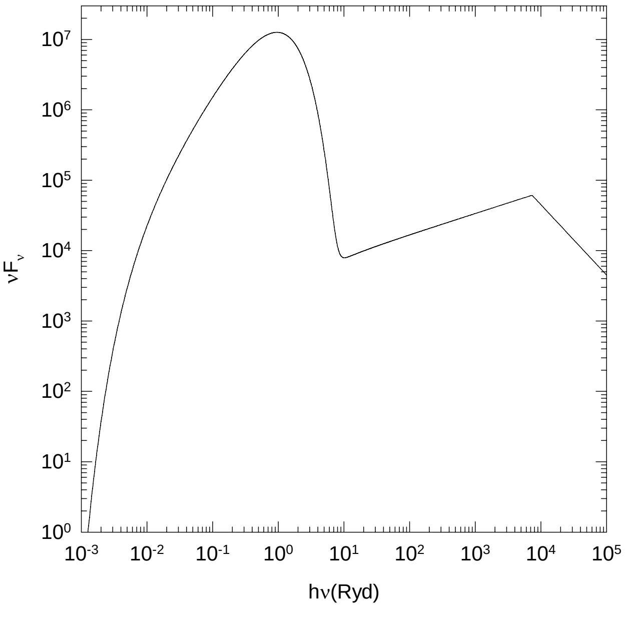


Figure 4 The continuum produced by the AGN continuum command. The Big Bump peaks at ≈1 Ryd, while the X-ray power law dominates at high energies. The two components are normalized by the second parameter, the value of α_{ox}. agncon

6.3. background, z=1.825, [f=100; no CMB]

This specifies a continuum shape and intensity chosen to mimic the cosmic radio to X-ray background (Ostriker & Ikeuchi 1983, Ikeuchi & Ostriker 1986, and Vedel, Hessten, & Sommer-Larsen 1994). Their ultraviolet continuum shape is an α = -1 power-law, with a mean intensity J_ν at 912Å given by

$$4\pi\, J_\nu\left(912\text{Å}\right) = 4\pi \times 10^{-21} \left(\frac{1+z}{3.5}\right)^4 \quad f$$

[erg Hz^{-1} cm^{-2} s^{-1}]

where *z* is the redshift and *f* an optional scale factor entered as the second parameter. Its default value is *f* = 1, and *z* = 0 (i.e., now) is assumed if no redshift is entered. Judging from Bechtold et al. (1987), Bajtlik, Duncan, and Ostriker (1988), and Vedel, Hessten, & Sommer-Larsen (1994), *f* is confidently known to be within an order of magnitude of unity.

This command specifies *both* the shape and intensity of the continuum. It is important that any previously occurring ordered pairs of shape and intensity commands be complete before this command is given.

Cosmic microwave background radiation is included in the generated background. This radiation field is assumed to be a blackbody radiation field, in strict thermodynamic equilibrium, with temperature given by

$$T_{CMB} = T_o\left(1+z\right) \quad [\mathrm{K}] \qquad (18)$$

where the redshift dependence is from Peebles (1971) and the present temperature of the background is assumed to be T_o = 2.725 ± 0.002K (Mather et al. 1999; Wilkinson 1987). This background can be an important source of Compton cooling for low-density clouds. If the optional keyword **no CMB** appears on the line then the background due to the CMB will not be included.

Thermal background radiation can also be specified independently with the **CMB** command, described on page 33 below.

The **table HM96** command (see page 39 below) uses a more sophisticated form of the energetic continuum, but only at a redshift of *z* = 2. The **table HM05** command (see page 40 below) works at any redshift.

This command does not add the cosmic-ray background. They should be included if the simulation is to extend into molecular gas. This is done separately with the **cosmic rays** command (page 104 below).

This radiation field is assumed to be isotropic rather than beamed.

6.4. blackbody t=100,000 [linear, _log, luminosity]

The continuum will be a blackbody with temperature (K) given by the number. The temperature may be entered directly or as a log. The number is assumed to be a log if it is less than or equal to 10 and linear if greater than 10. The keywords **_log** and **linear** will over ride this default and force the interpretation of the numbers to be either a log or linear. Embedded commas can improve readability, such as

```
black body, Temp = 1,000,000K
```

which is equivalent to

```
black 1000000
```

or

```
black body t=6  .
```

6.4.1. Peter Martin's blackbody luminosity options

The luminosity of the black body can be specified with command-line options. (P.G. Martin added these options.) If the luminosity is specified with any of these options then it must not also be specified with another luminosity command for this continuum source. The keywords that can appear on the line are given in the following subsections.

6.4.2. blackbody 5, luminosity = 38.

If the keyword **`luminosity`** appears then the second number is the log of the *total* luminosity (erg s^{-1}) of the black body, $4\pi R_{star}^2 \sigma T_{eff}^4$. This example would be a 10^5 K planetary nebula nucleus at the Eddington limit.

This is a luminosity command.

6.4.3. blackbody 5, radius = 10.

The log of the radius (in cm) of the blackbody R_{star} is used to set the total luminosity when the keyword **`radius`** appears. The total luminosity is $4\pi R_{star}^2 \sigma T_{eff}^4$. This example is also typical of a planetary nebula nucleus.

This is a luminosity command.

6.4.4. blackbody 50,000K, energy density = 500K.

The energy density of the blackbody radiation field, expressed as the equivalent blackbody temperature T_u in degrees Kelvin, is used to set the luminosity when the **`energy density`** keyword appears anywhere on the line. The energy-density temperature is defined from Stefan's law and the energy density of the radiation field u [erg cm^{-3}]:

$$T_u \equiv \left(\frac{u}{a} \right)^{1/4} \text{ [K]} \qquad (19)$$

where a is the Stefan's radiation density constant.

Both temperatures are interpreted as logs if they are less than or equal to 10 and linear otherwise. They will be interpreted as the linear temperature rather than as a log if the keyword **`linear`** appears. Note that if the **`linear`** key is used then both temperatures are interpreted as linear. Note also that the cosmic background radiation should also be included if $T_u \le 2.725\ (1+z)$ K. Cloudy will complain, but compute the model, if the energy density of the incident continuum corresponds to a temperature less than the present energy-density temperature of the universe.

This is an intensity command.

6.4.5. *blackbody, t = 50,000K, _STE*

The keyword **_STE**[10] (note the leading space) with no second number is equivalent to the **energy density** option with T_u set to the color temperature of the radiation field. This is a quick way to check that ionization and level populations go to strict thermodynamic equilibrium in the high radiation-density limit.

This is an intensity command.

6.4.6. *blackbody, t = 100,000K, dilution factor = -14*

Here the second parameter is the dilution factor *W* defined as

$$W \equiv \frac{J_\nu}{B_\nu} \approx \frac{\pi R_{star}^2}{4\pi r_o^2} \quad , \tag{20}$$

where R_{star} is the radius of the star and r_o is the separation between the illuminated face of the cloud and the center of the star. The approximation on the RHS assumes that R_{star} ? r_o. The dilution factor can be entered either directly or as a log (if the latter, then it will be negative). The example above is a rough approximation of the radiation field within a typical planetary nebula.

This is an intensity command.

6.5. bremsstrahlung, temp = 8

The continuum will be optically thin pure hydrogen bremsstrahlung emission. The shape is given by

$$f_\nu \propto \nu^{-0.2} \exp\left(-h\nu / kT\right) \quad [\text{erg cm}^{-2}\ \text{s}^{-1}\ \text{Hz}^{-1}]. \tag{21}$$

The argument is assumed to be the log of the temperature if it is less than or equal to 10 and linear otherwise. The form of the continuum is approximate since a simple power-law gaunt factor is assumed and the emission from an optically thin gas with cosmic abundances is actually characterized by hundreds of overlapping emission lines (see, for example, Kato 1976).

A more realistic continuum could be produced by combining the **coronal equilibrium** command (page 104 below) with the **punch transmitted continuum** command (page 148 below) to generate a continuum which can be read in with the **table read** command (page 42 below).

6.6. CMB [redshift 1000]

This command generates a blackbody radiation field in strict thermodynamic equilibrium (that is, $T_{color} = T_u$, where T_u is the energy-density temperature). The optional argument is the redshift *z*. If it is not entered then *z* = 0 is assumed. The temperature of the blackbody is given by

[10] The keyword was **LTE** before version 96 of the code. It was changed to **STE** to better reflect the fact that this condition corresponds to strict thermodynamic equilibrium. The code will continue to accept the **LTE** keyword for the foreseeable future.

$$T_{CMB} = T_o(1+z) \quad \mathrm{K} \tag{22}$$

where the redshift dependence is from Peebles (1971) and the present temperature of the background is assumed to be T_o = 2.725±0.002K (Mather et al. 1999; Wilkinson 1987). This command specifies *both* the shape and intensity of the radiation field. A starting radius of 10^{30} cm will be assumed if no starting radius is specified.

This radiation field is assumed to be isotropic rather than beamed.

6.7. extinguish column = 23, leak = 0.05, low =4 Ryd

This command will modify the shape of the continuum by extinction due to photoelectric absorption by a cold neutral slab with column density given by the first argument (entered as a log, cm^{-2}). This occurs *after* the continuum has been fully generated and normalized to the correct intensity. The form of the extinction is a simple power-law fit to the absorption curves calculated by Cruddace et al. (1974). The extinguished continuum f_ν' is related to the initial continuum f_ν by

$$f_\nu'(\nu \geq 1\,\mathrm{Ryd}) = f_\nu \left\{ \eta + (1-\eta)\exp\left(-6.22\times 10^{-18}\,\nu_{Ryd}^{-2.43}\,N(\mathrm{H})\right)\right\} \tag{23}$$

where N(H) is the total hydrogen column density (cm^{-2}), ν_{Ryd} is the frequency in Rydbergs, and η is the leakage.

The optional second number is the fractional leakage η through the absorber (see Ferland and Mushotzky 1982). This has a default value of 0, i.e., no leakage. The leakage is interpreted as a log if it is negative and linear otherwise. If unexpected or unphysical results occur when the **`extinguish`** command is given then it is likely that nearly all ionizing radiation has been attenuated. A plot of the generated continuum (with the **`plot continuum`** command) may prove interesting. The code will stop if the leakage is greater than 1.0 (100%).

The optional third number is the lowest energy for the absorption to occur. The default is 1 Ryd and is appropriate if the absorption is mainly due to hydrogen. The number is interpreted as linear Rydbergs if positive and the log of the energy if less than or equal to zero. The continuum with energies below this cutoff energy will be unaffected by the absorption. The non-ionizing ($h\nu$ < 1 Ryd) continuum can be extinguished by this command but extrapolating the power law to these energies is nonsense.

The second two arguments are optional and may be omitted from right to left. The cutoff energy can only be changed if the leakage is specified.

The command acts by first generating the continuum shape with extinction neglected. The continuum is then normalized using any of the luminosity or intensity commands (i.e., **`Q(H)`**, **`ionization parameter`**, **`luminosity`**, etc.). Only *then* is the continuum extinguished. The continuum that actually strikes the illuminated face of the cloud *does not* have the intensity or luminosity actually entered. (These values would be correct were the extinction not present.) Physically, the luminosity of the central object is not changed by the presence of an absorbing cloud along the line of sight.

This command should not be used except as a quick test. A more physical way to extinguish the continuum would be to actually transmit it through a model of the absorbing slab, save that continuum with the **`punch transmitted continuum`** command (page 148 below), then use this filtered continuum with the **`table read`** command (described on page 42 below).

6.7.1. extinguish optical depth 1.2, [options]

If **`optical depth`** appears rather than **`column`** then the first number is the log of the optical depth. All other options are the same as the **`extinguish column`** command. ***N.B.*** it really is the log of the optical depth, not the linear optical depth.

6.8. fireball [redshift = 2000]

This command is replaced with the **`CMB`** command, described on page 33 above.

6.9. interpolate [ν(Ryd) or log ν(Hz)], log(f_ν)

The continuum shape will be interpolated from the table of points given by this command. The interpolation uses straight lines in log-log space. Up to 130000 ordered pairs of points can be entered. This limit is set by the variable ***NCELL***, which also sets the size of several continuum arrays. **`continue`** lines can be used to continue entering values after the initial **`interpolate`** line is filled.

Unlike the majority of the commands the first five characters of the command must be entered.

The numbers are ordered pairs giving the energy and intensity. The first number within each ordered pair of points is *either* the energy in Rydbergs (linear or as a log) *or* the log of the frequency (in Hertz). Cloudy assumes that the log of the energy in Rydbergs was entered if the first number is negative; that the log of the frequency (Hz) was entered if the first number is greater than 5; and linear Rydbergs otherwise. Any of the three styles can be chosen but it must be used consistently within the command. If the first energy is entered as zero then it is interpreted as the low-energy limit of the code. In this case the remaining energies will be interpreted as linear Rydbergs if the second number is positive and the log of the energies in Rydbergs if it is negative. An energy of zero Rydbergs is not allowed (except for the first), and the energies must be in increasing order.

The second number in each ordered pair is the log of the relative flux density per unit energy interval [$\log_{10}(J_\nu)$+constant] at that energy. These numbers are only used to set the shape of the continuum. The constant in the equation is set by one of the intensity or luminosity commands.

The **`interpolate`** command can be freely mixed with other continuum shape commands and a total of up to 100 **`interpolate`** and **`table`** (see 37 below) commands can be entered.[11] Note that **`table`** and **`interpolate`** are actually two

[11] Limits to the use of the **`interpolate`** command existed in versions 73 and before, but have been lifted.

forms of the same command so that they store information in the same arrays. The total number of **table** and **interpolate** commands entered together cannot exceed 100.

As an example, the following approximates a metal-poor 45,000 K stellar atmosphere. The energies are entered in Rydbergs:

```
// following is 45000 K atmosphere from Shields and Searle
interpolate (0.00001 -11.106) (.58 -1.5792) (.99 -1.44) (1.01 -1.7018)
continue  1.8 -1.905) (1.81 -1.939) (2.57 -2.208) (2.59 -2.247) (3 -2.3994)
continue (3.02 -2.8193) (3.49 -2.9342) (3.51 -4.143) (3.99 -5.582)
continue (4.01 -6.3213) (6 -9.9) (10 -17.3) (20 -30) (10,000,000 -30)
q(h) = 52.778151
```

Note that the continuum should be specified between 1.001×10^{-8} Ryd and 7.354×10^{6} Ryd even if the intensity is small. If it is not fully specified then a warning will be issued and a model computed with the unspecified continuum set to zero. As a further note, it is important that the continuum be physically correct. For instance, stellar model atmospheres predict almost no X-ray emission while real OB stars *are* X-ray sources (although neglecting X-rays for these stars is generally a safe approximation). See page 44 below for a further discussion.

6.10. laser, frequency = 3.5 Ryd [rel width 0.02]

The intensity of the continuum will be very small except within ±5% of the specified energy where it will be very large. The energy is specified in Rydbergs and it is interpreted as a log if it is negative. This is provided as a way to check on the computation of the photoionization rate integrals.

The optional second number changes the relative width of the laser. The relative width is the ratio *dE/E* where *dE* is the half width of the laser. The laser will only be active within ± *dE* of *E*. The code would return an error condition if *dE* is so small that the laser does not happen to be within ± *dE* of *E* as evaluated by the code's energy mesh. The fractional width probably should not be made smaller than roughly 0.01 but the code does not protect against too small a value of *dE*.

Another way to make a laser is to punch out a transmitted continuum, edit this file, and, by hand, increase the intensity of the continuum at particular cells. This is described where the **table read** command is defined (page 42 below).

6.11. power law, slope =-1.4 [hi cut =6 Ryd low cut =.1, Kelvin]

N.B. IT IS VERY DANGEROUS TO USE THIS COMMAND. The continuum will be a power law with slope given by the first parameter. It has optional low-energy and high-energy exponential cutoffs $\nu_{high\ cut}$ and $\nu_{low\ cut}$ in Rydbergs. The form of the continuum is

$$f_{\nu} = \nu^{+\alpha} \exp\left(-\nu / \nu_{high \quad cut}\right) \exp\left(-\nu_{low \quad cut} / \nu\right) \quad [\mathrm{erg\ cm^{-2}\ s^{-1}\ Hz^{-1}}]. \qquad (24)$$

The first number on the command line is the slope α. Note that there is no implicit negative sign in this exponent; typical AGN have α_{ox}~ -1.4, (Zamorani et al. 1981). The second (optional) number is the high-energy cutoff $\nu_{high\ cut}$. The third optional number is the low-energy cutoff $\nu_{low\ cut}$. Both are expressed in Rydbergs, and can be omitted from right to left. The default values are 10^4 and 10^{-4} Ryd.

If the keyword **`Kelvin`** appears then both cutoff energies are interpreted as temperatures in Kelvin rather than energies in Rydbergs. The temperature is a log if it is less than or equal to 10 and the linear temperature itself if greater than 10.

It is generally a *very bad* idea to use this command. Cloudy treats the entire continuum between *very* low and *very* high energies. Extrapolating reasonable continua past the optical-ultraviolet region into radio or γ-ray energies will have unexpected effects. Power-law continua with slopes smaller than -1 will have unphysically large photon occupation numbers and brightness temperatures at very long wavelengths. This will probably produce catastrophic Compton cooling and/or free-free heating. Continua with slopes greater than -1 will be dominated by the radiation field at energies of many MeV, resulting in large Compton heating and pair production rates. The exponential cutoffs can prevent this but they also drive the continuum to zero intensity when either argument in the exponential becomes large. This is unphysical and can cause numerical problems.

It is *much* better to use the **`interpolate`** command (page 35 above), and enter physically reasonable low-energy and high-energy continua. There is a special version of the command, **`table power law`** described on page 41 below, for entering a well-behaved power-law continuum.

6.12. table command

6.12.1. Overview

Any of several continuum shapes that are stored as a permanent part of the code can be entered with this command. This is a special version of the **`interpolate`** command, described on page 35 above. The same interpolation on a table of input frequencies and fluxes described there is done. The **`table`** command can be freely mixed with other shape commands and a total of up to 100 **`table`** and **`interpolate`** commands can be entered.

6.12.2. table _agn

If the keyword **`_agn`** appears (note the presence of a leading space) then a continuum similar to that deduced by Mathews and Ferland (1987) will be used. The continuum is meant to be similar to typical radio quiet active galaxies. The points used to describe this continuum are given in Table 4.

Table 4
AGN Continuum

ν(Ryd)	log (F_ν)	slope
1.00(-5)	-3.388	+2.50
9.12(-3)	4.0115	-1.00
0.206	2.6576	-0.50
1.743	2.194	-1.00
4.130	1.819	-3.00
26.84	-0.6192	-0.70
7.35(+3)	-2.326	-1.67
7.40(+6)	-7.34	-

This continuum differs from the Mathews and Ferland (1987) continuum only in that the continuum is assumed to have a sub-millimeter break at 10 microns. For wavelengths longer than 10 microns the continuum is assumed to have a slope $f_\nu \propto \nu^{+2.5}$, appropriate for a self-absorbed synchrotron continuum (Rybicki and Lightman 1979). Note that this represents a typical observed continuum, and may not be directly related to the continuum actually striking BLR gas (Korista, Baldwin, and Ferland 1997).

Table 5

Akn 120 Continuum

ν(Ryd)	f_ν
1.0(-5)	1.5(-26)
1.9(-5)	1.6(-26)
3.0(-4)	1.4(-23)
2.4(-2)	8.0(-25)
0.15	1.6(-25)
0.30	1.8(-25)
0.76	7.1(-26)
2.0	7.9(-27)
76.	1.1(-28)
7.6(+2)	7.1(-30)
7.4(+6)	1.3(-34)

The energy of the sub-millimeter break is not well determined observationally but has a major impact on high density, high ionization parameter models, as discussed by Ferland and Persson (1989), Ferland et al. (1992), and Ferland (1999a). The energy of the infrared break can be adjusted with the **break** keyword. The break can be adjusted between the limits of 0.2 Rydberg and 1.001×10^{-8} Ryd by entering the keyword **break** followed by a number specifying the energy of the break. The number is interpreted as the log of the energy in Rydbergs if it is negative and as linear Rydbergs if positive. It is interpreted as the linear wavelength of the break in microns if the keyword **microns** also appears. If no number appears, but the keywords **no break** does, then a break at the low-energy limit of the code (1.001×10^{-8} Ryd) is assumed. The following shows equivalent ways of generating a continuum with a break at 10 microns;

```
table AGN break .00912  // energy in Ryd
table AGN break -2.04   // log of energy in Ryd
table AGN break 10 microns // wavelength in microns
table AGN no break      // no sub-millimeter break
```

Note that the nature of the continuum in AGN is still an open question. The continuum given here is very simplistic and quite uncertain in the ionizing ultraviolet. Moreover, it would not be surprising if the BLR sees a far different continuum than we do. This continuum may not be correct for low redshift Seyfert galaxies (Binette et al. 1989; Clavel and Santos-Lleo 1990) and direct observations of high-redshift quasars suggest a far softer continuum than this (Zheng et al. 1997; Korista, Ferland, & Baldwin 1997). It is probably best to only use this continuum in exploratory situations, and to generate a specific AGN continuum using either the **ratio** command described on page 27 above or the **agn** command described on page 29 above.

6.12.3. table akn120

If the keyword **akn120** appears then the continuum summarized by Peterson et al. (in preparation) is used. The continuum is described by the observed flux at Earth [erg cm^{-2} s^{-1} Hz^{-1}] and is given in Table 5.

The monochromatic luminosity at 1320 Å is νL_ν=1.84 ×10^{44} h^{-2} erg s^{-1}, where $h \equiv H_o/100$ km s^{-1} mpc^{-1}, so, setting h = 0.75, the **akn120** continuum could be generated by the commands

```
nul(nu) = 44.514 at 0.6906 Ryd
table akn120
```

6.12.4. *table cooling flow*

The keyword **`cool`** generates the continuum shape described by Johnstone et al. (1992) and used in Ferland, Fabian, & Johnstone (1994; 2002). It is a co-added series of Raymond-Smith collisional-equilibrium continua and was chosen to represent the spectrum at a point within a typical cooling flow.

6.12.5. *table crab*

This gives the continuum summarized by Davidson and Fesen (1985). This is the net observed continuum, originating in both the pulsar and nebula, and not the pulsar continuum alone. The continuum is given in Table 6, which gives the observed flux at Earth (erg cm^{-2} s^{-1} Hz^{-1}).

According to Davidson and Fesen, the total luminosity of the Crab is L_{tot} = 10$^{38.14}$ erg s^{-1}. The Crab continuum could be generated by combining the commands

```
luminosity (total) 38.14
table Crab
```

Table 6
Crab Continuum

ν(Ryd)	f_ν
1.0(-5)	3.77E-21
5.2(-4)	1.38E-21
1.5(-3)	2.10E-21
0.11	4.92E-23
0.73	1.90E-23
7.3	2.24E-24
73.	6.42E-26
7.3(+3)	4.02E-28
1.5(+6)	2.08E-31
7.4(+6)	1.66E-32

6.12.6. *table Draine [factor=1.7]*

This enters the galactic background radiation field given by equation 23 of Draine & Bertoldi (1996). The continuum is only defined over a very narrow wavelength range so it is only appropriate for certain simple PDR calculations. It is shown in Figure 5 along with the continuum produced by the **`table ism`** command. This command specifies both the shape and intensity of the continuum. The optional scale factor changes the intensity of the continuum.

This continuum is defined up to an energy very close to 1 Rydberg. It may spill over into the hydrogen-ionizing continuum for certain choices of the continuum bin resolution. Add the **`extinguish`** command, described on page 34 above, to insure that H-ionizing radiation is extinguished if this is needed. The code will print a comment is this is not done.

This continuum should only be used for restricted tests since the vast majority of the electromagnetic spectrum is undefined. It was created to compute the Leiden PDR test cases (the *pdr_leiden** simulations in the test suite) and the paper by Röllig et al. (2007).

This radiation field is assumed to be isotropic.

6.12.7. *table HM96 [factor=-1]*

This enters the Haardt & Madau (1996) background continuum for a redshift of z = 2.16. This is the original form of the command and is maintained for reference. The cosmic microwave background is not included – use the **`CMB`** command described on page 33 above to add this component. Note that this table specifies both the shape and intensity of the continuum. There is an optional multiplicative scale factor to change the intensity. If the scale factor is less than or equal to zero then it is interpreted as the log of the scale factor.

This radiation field is assumed to be isotropic rather than beamed.

6.12.8. table HM05 redshift 2.21 [quasar; factor=-1]

This enters the Haardt & Madau (2005 in preparation) continuum at any redshift 0 ≤ z ≤ 8.9. It interpolates on tables kindly provided by Francesco Haardt. There are two forms of the continua – the default includes both quasars and galaxies. If the keyword **`quasar`** occurs then a continuum considering only quasars is used. The cosmic microwave background is not included – use the **`CMB`** command described on page 33 above to add this component. Note that this table specifies both the shape and intensity of the continuum. There is an optional multiplicative scale factor to change the intensity. If the scale factor is less than or equal to zero then it is interpreted as the log of the scale factor.

This radiation field is assumed to be isotropic rather than beamed.

6.12.9. table _ism [factor = 0.7]

The local interstellar radiation field is generated with the keyword **`_ism`**. This

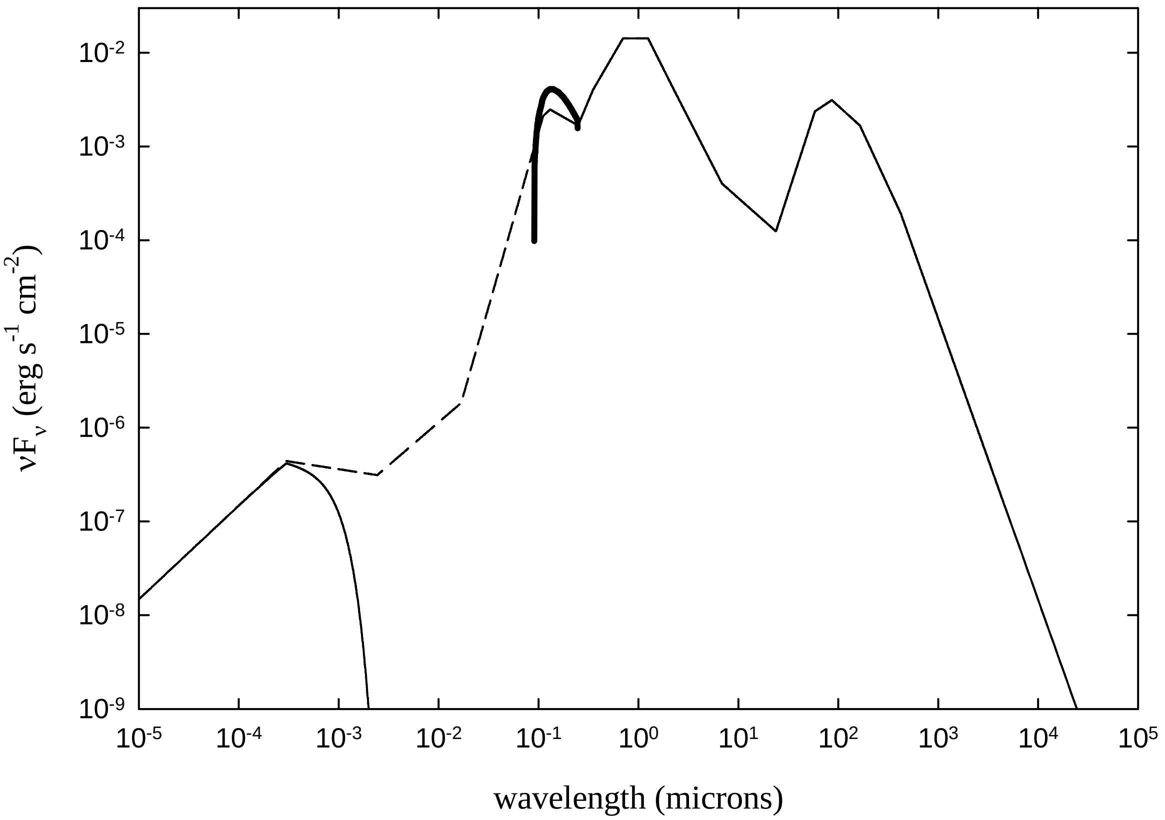


Figure 5 The continuum produced by the **`table ISM`** command is the lighter line. The infrared cirrus is the peak at λ ~ 100 μm and starlight dominates at shorter wavelengths. The points just shortward of the Lyman limit (0.0912 μm) are interpolated – actually it is thought that interstellar extinction removes most of this continuum. The dashed line shows the interpolated continuum and the solid line shows the effects of absorption introduced by adding the **`extinguish`** command. The heavy line is the **`table Draine`** continuum. Ism_background

uses Figure 2 of Black (1987) to represent the *unextinguished* local interstellar radiation field (see Figure 5). This command specifies *both* the shape and luminosity of the radiation field. The continuum generated by Cloudy is exactly that given by Black except that the radiation field between 1 and 4 Ryd is interpolated from the observed or inferred values. Actually it is thought that this part of the radiation field is heavily absorbed by gas in the ISM so that little 1 to 4 Ryd radiation exists, at least in the galactic plane. Such absorption can be introduced with the **`extinguish`** command, described on page 34 above.

Table 7
ISM Radiation Field

log(ν)	log ν f_ν	log ν	log νf_ν
9.00	-7.93	14.14	-2.30
10.72	-2.96	14.38	-1.79
11.00	-2.47	14.63	-1.79
11.23	-2.09	14.93	-2.34
11.47	-2.11	15.08	-2.72
11.55	-2.34	15.36	-2.55
11.85	-3.66	15.54	-2.62
12.26	-2.72	16.25	-5.68
12.54	-2.45	17.09	-6.45
12.71	-2.57	18.00	-6.30
13.10	-3.85	23.00	-11.30
13.64	-3.34		

The **`table ism`** command also specifies the intensity of the incident radiation field since this is directly observed. There is an optional scale factor to change the intensity of the entire radiation field. It is the log of the scale factor if less than or equal to zero and the scale factor itself if positive. The actual numbers used by Cloudy to interpolate on Black's table are given in Table 7. The frequencies are in Hz, and the product νf_ν in erg cm^{-2} s^{-1}.

This does not include the cosmic microwave background. Use the **`CMB`** command described on page 33 above to add this component.

The actual ISM radiation field incident on a typical region in the galactic plane could be generated by:

```
table ISM
CMB
extinguish column = 22 leak=0
```

This radiation field is assumed to be isotropic rather than beamed.

6.12.10. table power law [spectral index -1.4, low =.01, hi =20]

This produces a power-law continuum that is well behaved at both the high and low energy ends. The default shape, assumed when no numbers occur on the command line, is the form $f_\nu \propto \nu^\alpha$. Here α = -1 for the spectral midrange between 10 microns and 50 keV, and the continuum has slopes $f_\nu \propto \nu^{5/2}$ at lower energies (appropriate for self-absorbed synchrotron, eq 6.54, p.190, Rybicki & Lightman 1979) and $f_\nu \propto \nu^{-2}$ at higher energies. Note that much of the X-ray literature will use an implicit negative sign in defining the energy index, as in equation 13.2 of AGN3. Cloudy never uses implicit negative signs so a typical AGN will have an energy index of roughly -1.5. Table 8 summarizes the continuum that is produced by this command if no other parameters are specified.

Three optional numbers may appear on the command line. The first number sets the slope of the mid-range spectral component (infrared to X-ray) and has a default of -1 ($f_\nu \propto \nu^{-1}$).

The next two numbers adjust the energy limits of the mid-range spectral component. Their default units are Rydbergs but the keyword **microns** will change the units to microns *for the first energy only*. The second number is the energy (in Rydbergs) of the infrared break. The default is 0.009115 Ryd (10 microns). If this second number is zero then the low energy limit to the continuum (1.001×10^{-8} Ryd) will be used. The number is interpreted as the log of the energy in Rydbergs if it is negative and linear otherwise. Note that, with no infrared break, free-free heating will probably be significant for denser clouds. A power-law continuum with a low energy break at 1 micron would minimize this heating and could be generated with the command

Table 8
Power Law
Continuum

ν(Ryd)	slope
1.00(-8)	+2.50
9.115(-3)	-1.00
3676.	-2.
7.40(+6)	-

```
// a power-law with index -1 and 1 micron break
table power law slope -1, 1 micron break
```

This uses the default continuum

```
// another example, a power-law with index -1 and 10 micron break, the default
table power law slope -1
```

The third optional number is the energy (in Rydbergs) of the break in the X-ray continuum. The default is 50 keV, and if it is zero then the high-energy limit of the continuum (7.354×10^{6} Ryd) is used. The number is interpreted as a log if the energy of the infrared break is entered as a log and linear otherwise. The numbers may be omitted from right to left.

6.12.11. table read "contin.txt"

This reads in the continuum predicted from a previous Cloudy calculation. The name of the file containing the previous continuum must be enclosed in a pair of double quotes. The first calculation saves the continuum transmitted through a cloud with the **punch transmitted continuum** command. Subsequent calculations use the **table read** command to include this continuum.

The **punch transmitted continuum** command is described on page 148 below. It produces a file containing the frequency in Rydbergs and the transmitted continuum νf_ν (erg cm^{-2} s^{-1}). This continuum is the sum of the attenuated incident continuum and the fraction of the diffuse emission from the cloud that is transmitted in the outward direction. The first line of the input file contains header information and must not be deleted.

The keyword **last** must appear on the **punch transmitted continuum** command if more than one iteration is done. If it does not then the continuum from each iteration will be punched and the code will become confused when it tries to read the file.

The **`table read`** command can be freely mixed with all of the other continuum shape commands. Any number of **`table read`** commands can be entered[12]. The continuum file must have been produced by the same version of Cloudy. The code will stop if otherwise.

This does not set the intensity of the continuum. This must be done with any of the intensity or luminosity commands.

The following gives an example of first creating a file containing the transmitted continuum then using this file as the continua in a second calculation.

```
title this finds transmitted continuum due to warm absorber
hden 9
ionization parameter 1
stop effective column density 21
table AGN
iterate
punch transmitted continuum file = “absorber.txt” last
```

Now use this continuum in a second calculation:

```
table read file = “absorber.txt”
luminosity 45
radius 18
hden 9
```

6.12.12. table Rubin

Nearly all attempts at modeling the Orion Nebula have found that theoretical stellar atmospheres do not produce enough flux near 4 Ryd (see, for example, Mathis 1982, 1985; Rubin et al. 1991; Sellmaier et al. 1996).

Bob Rubin has modified the emergent continuum from one of the Kurucz (1979) models to better account for the presence of high ionization lines in the Orion Nebula. This modified continuum can be accessed with the **`table Rubin`** command. The continuum started life as a log g = 4, T_{eff} = 37,000 K Kurucz model, but the flux between 41 eV and 54 eV was raised by a factor of 11 to reproduce the [Ne III] optical and IR lines.

6.13. table starburst age=6.7 “data.txt”

It is possible to read in predictions from Starburst 99 (Leitherer et al. 1999). This command, which existed in versions through C07, has been replaced. The Starburst 99 SEDs have been unified with the stellar atmosphere treatment. The procedure is to store the Starburst output in a file with a “*.stb99*” or “*.stb*” extension and compile it

```
compile star "some_file.stb99"
```

This will produce files *some_file.ascii* and *some_file.mod*, which can then be used in the **`table stars`** command:

```
table star "some_file.mod" age=6.7
```

[12] Only one table read command could be entered in versions 90 and before.

Multiple starburst SEDs can be combined. The **`table stars`** command is described next.

It is critical that the original Starburst 99 file not be changed in any way at all. Doing so will trick the code into generating bogus results. In any case, it is a good idea to make a plot of the generated continuum, using column 1 and 2 of the output from the **`punch continuum`** command, described on page 143 below, to confirm that it is correct.

This radiation field is assumed to be isotropic rather than beamed.

6.14. table stars overview

Several sets of emergent SEDs from stellar atmosphere calculations are accessible. The command has several sub-keywords that indicate which set of atmospheres to use.

Figure 6 compares predictions for five of the 50,000 K SEDs that are available. These include a blackbody and atmospheres computed by Mihalas (1972), Kurucz (1979), Kurucz (1991) and Rauch (1997). All were normalized to have the same total luminosity (10^{38} erg s^{-1}) observed from a distance of 10^{18} cm. Note the order of magnitude dispersion among the continua for energies around 4 Ryd.

These commands specify only the continuum shape. It is still necessary to specify a luminosity. Tout et al. (1996) provide convenient fitting formulae giving zero age main sequence luminosities as functions of stellar mass and metallicity.

6.14.1. A high-energy component?

Theoretical stellar atmospheres emit little energy above 4 Ryd while real OB stars *are* X-ray sources. Sciortino et al. (1990) find a correlation between the X-ray and bolometric luminosities which can be fitted by

$$\log\left(L_x\right)=1.08\left(+0.06/-0.22\right)\log\left(L_{bol}\right)-9.38\left(+2.32/-0.83\right) \quad . \qquad (25)$$

The X-ray luminosity is typically ;6.4 dex fainter than the bolometric luminosity. A source temperature of 0.5 keV is quoted by Sciortino et al. This X-ray continuum must be explicitly added as an independent continuum source. Tests show that the high-energy light has little effect on conditions in the H II region but *does* affect the ionization in the surrounding PDR.

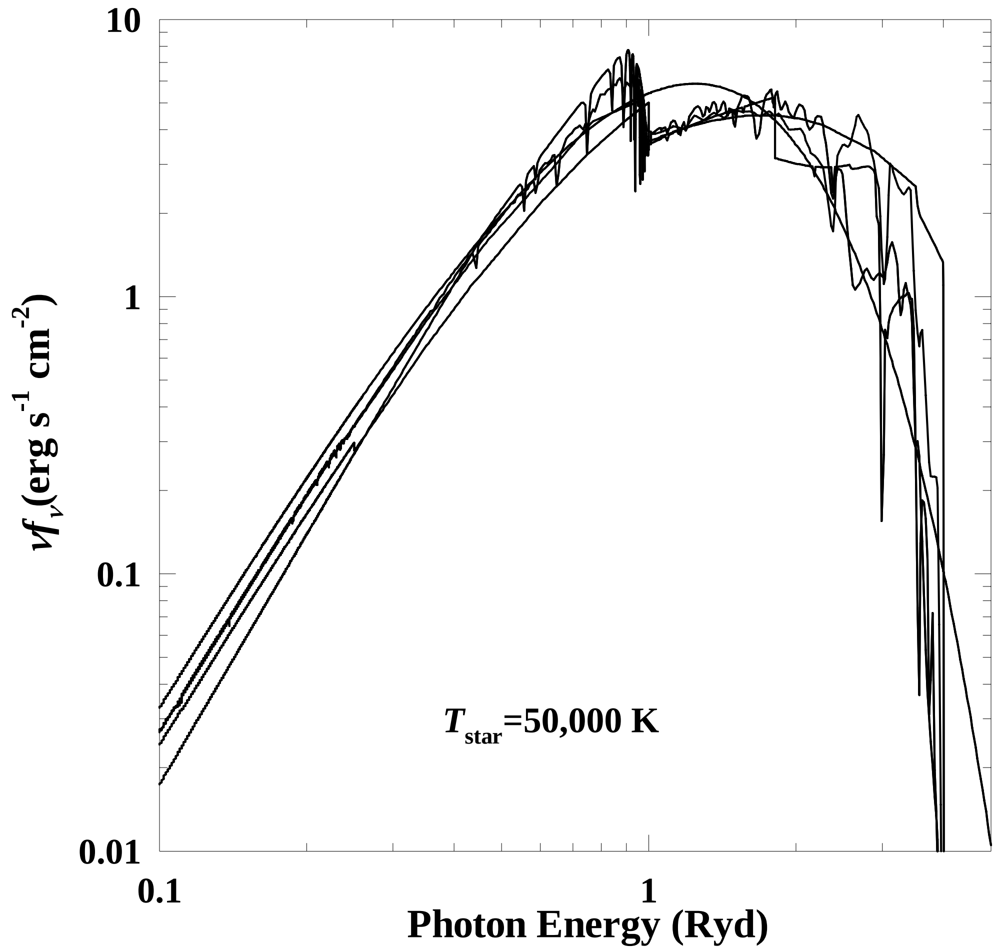


Figure 6 This figure shows the emergent continua predicted by five 50,000 K stars included with the code. The smoothest is the blackbody, and the Kurucz (1991) and Rauch (1997) atmospheres show the most structure. stars

6.14.2. *Overview of available stellar continua*

In versions C06.02 and before the stellar continua were entered into the code on a case by case basis. New continua could only be introduced by writing new code. Beginning in C07.02 Peter van Hoof developed a unified treatment so that any continuum could be used by putting it into a standard format. This is far more flexible and allows more continua to be entered. The descriptions of the available continua are now kept on the web site. This allows more continua to be added without requiring changes to this document. The following gives a brief sketch of some of the continua that are available at the time of this writing.

All grids have a range of surface temperature and many also include a range of abundances and surface gravities. The command will interpolate on these tables to find a continuum with a specified parameters.

The following only lists some of the available continua and is probably out of date. The web site http://wiki.nublado.org/wiki/StellarAtmospheres is up to date and gives much more information.

table star Kurucz These are subsets of the Kurucz (1979; with supplements) line-blanketed LTE atmospheres. A range of temperatures is available.

table star Mihalas These are subsets of the Mihalas (1972) non-LTE OB stellar atmospheres. A range of temperatures is available.

table star atlas, temp =40,000 [log(g)=4.5] These are the Kurucz (1991) grid. A range of temperatures and gravities are available.

table star Rauch, temp=100,000 [halo log(g)=6.5] These are the first generation Rauch (1997) and second generation Rauch (2002) grids of non-LTE model planetary nebula nuclei. The grid includes a range of temperatures, gravities, and two abundance sets.

table star Werner, temp =140,000 [log(g)=7.4] This is the Werner and Heber (1991) grid of non-LTE model planetary nebula nuclei atmospheres. The grid includes a range of temperatures and gravities.

table star CoStar, temp=34,700K log(g)=4 [index 2, ZAMS, age] This uses the CoStar (Schaerer et al. 1996a, b; and Schaerer & de Koter 1997) grid of windy hot stellar atmospheres. There are many possible ways, described next, to interpolate on this grid. Two abundance sets exist. If the keyword **halo** appears then the halo abundance set will be used. If no keyword appears, or the keyword **solar** appears, then the solar set will be used.

table star CoStar, 37,000K, index 2. The CoStar grid consists of 6 evolutionary tracks, each corresponding to a specific Zero Age Main Sequence (ZAMS) mass, and two abundance sets, solar and halo. Each evolutionary track consists of several models (ranging from 3 to 7, depending on the track). The index number of the model corresponds to a specific age of the star as it is followed through its evolution. So the index number is a rough way to indicate how evolved the star is; index 1 indicates a main sequence star, higher numbers indicate more evolved stars. If the keyword **index** appears then the index is the second optional number and the code will interpolate the temperature along this index.

If only one number is on the line and no keyword appears then an index of unity is assumed. It is possible to specify a ZAMS mass, surface gravity, or age with the following commands. The original CoStar file should be consulted to see what range of parameters is available.

table star Costar, 37,000 4. With no keyword the second parameter is the log of the surface gravity.

table star CoStar, ZAMS mass=30, time=1000000. With the **ZAMS** keyword the ZAMS mass and age of the star is specified.

table star CoStar, age=1000000, mass=30. With the **_AGE** keyword the mass and age of the star is specified.

7. CHEMICAL COMPOSITION

7.1. Overview

The default solar composition is summarized in Table 9. C and O abundances come from photospheric abundances of Allende Prieto et al. (2002, 2001), while N, Ne, Mg, Si, and Fe are from Holweger (2001). The helium abundance is a typical value for nebulae with near-solar compositions. The remainder of the first thirty elements comes from Grevesse & Sauval (1998). Meteoritic and photospheric abundances agree for most elements. They differ by significant amounts for P, S, Cl, and Mn. These are fairly volatile elements so may be deficient in meteorites. For these four the means of the meteoritic and photospheric abundances were used.

Table 9
Solar Composition

A			12+log	log	n/n(H)	ref
1	H	Hydrogen	12.00	0.00	1.00E+00	GS98
2	He	Helium	11.00	-1.00	1.00E-01	text
3	Li	Lithium	3.31	-8.69	2.04E-09	GS98
4	Be	Beryllium	1.42	-10.58	2.63E-11	GS98
5	B	Boron	2.79	-9.21	6.17E-10	GS98
6	C	Carbon	8.39	-3.61	2.45E-04	AP02
7	N	Nitrogen	7.93	-4.07	8.51E-05	H01
8	O	Oxygen	8.69	-3.31	4.90E-04	AP01
9	F	Fluorine	4.48	-7.52	3.02E-08	GS98
10	Ne	Neon	8.00	-4.00	1.00E-04	H01
11	Na	Sodium	6.33	-5.67	2.14E-06	GS98
12	Mg	Magnesium	7.54	-4.46	3.47E-05	H01
13	Al	Aluminium	6.47	-5.53	2.95E-06	GS98
14	Si	Silicon	7.54	-4.46	3.47E-05	H01
15	P	Phosphorus	5.51	-6.50	3.20E-07	GS98*
16	S	Sulphur	7.27	-4.74	1.84E-05	GS98*
17	Cl	Chlorine	5.28	-6.72	1.91E-07	GS98
18	Ar	Argon	6.40	-5.60	2.51E-06	GS98
19	K	Potassium	5.12	-6.88	1.32E-07	GS98
20	Ca	Calcium	6.36	-5.64	2.29E-06	GS98
21	Sc	Scandium	3.17	-8.83	1.48E-09	GS98
22	Ti	Titanium	5.02	-6.98	1.05E-07	GS98
23	V	Vanadium	4.00	-8.00	1.00E-08	GS98
24	Cr	Chromium	5.67	-6.33	4.68E-07	GS98
25	Mn	Manganese	5.46	-6.54	2.88E-07	GS98*
26	Fe	Iron	7.45	-4.55	2.82E-05	H01
27	Co	Cobalt	4.92	-7.08	8.32E-08	GS98
28	Ni	Nickel	6.25	-5.75	1.78E-06	GS98
29	Cu	Copper	4.21	-7.79	1.62E-08	GS98
30	Zn	Zinc	4.60	-7.40	3.98E-08	GS98

References: GS98: Grevesse & Sauval (1998), GS98* - mean of photospheric and meteoritic, H01: Holweger (2001), AP01, AP02 Allende Prieto et al. (2001, 2002).

Abundances are always specified by *number* relative to *hydrogen*, not by mass or relative to silicon. Abundances are relative to the total hydrogen density, the sum of H in atomic, ionic, and molecular form. These are gas phase abundances and do not include material locked into grains. The composition will be printed in the header information that starts the printout. You should check this to confirm that the right composition is used.

The following sections describe how to modify the chemical composition.

7.2. Absolute abundances and scale factors

Abundances can be specified as either *absolute abundances* or as *scale factors*. An absolute abundance gives the abundance of an element relative to hydrogen. An example might be $n(\mathrm{O})/n(\mathrm{H}) = 4 \times 10^{-4}$. A relative abundance is given relative to another value. An example might be the abundance relative to the solar value, $n(\mathrm{O})/n(\mathrm{H}) = 4 \times [n(\mathrm{O})/n(\mathrm{H})]_{/}$.

7.3. Precedence

If the absolute abundance is specified with more than one command then the last abundance is used. If the abundance is specified by both its absolute abundance and by a scale factor then both are used. Either of the following will multiply the default H II region nitrogen abundance by a factor of two:

```
abundances H II region
element scale factor nitrogen 2
```

or

```
element scale factor nitrogen 2
abundances H II region
```

The **element scale factor** option applies a scale factor while the **element abundance** option sets an absolute abundance. The **abundances H II region** command uses one of the absolute abundance mixtures that are stored by the code. These are listed in Table 10. This command enters the gas-phase abundances of all 30 elements and also includes interstellar grains. The **element** command changes some details about a particular element and is described further on page 54 below.

In the following example both commands set absolute abundances so the first nitrogen **abundance** will have no effect and the final nitrogen abundance will be the default H II region abundance

```
element abundance nitrogen -4.7
abundances H II region
```

In the following only the second nitrogen scale factor has any effect since the second scale factor overwrites the first:

```
element scale factor nitrogen 3
element scale factor nitrogen 2
abundances H II region
```

The result will be HII region abundances with nitrogen having twice its normal value. Similarly, the combination

```
element abundance nitrogen –4
element scale factor nitrogen 2
```

in either order would result in $n(\mathrm{N})/n(\mathrm{H}) = 2\times10^{-4}$ since the first command sets an absolute abundance of 10^{-4} and the second command doubles this.

The chemical composition is printed at the start of the calculation. Be sure to confirm that the composition has been entered correctly.

7.4. abundances he c . . .

The abundances of all elements can be entered with the command **abundances** followed by: a) a complete set of abundances, b) the keyword **_all** and a single number to set all of the abundances, or c) a second keyword to select one of the stored abundance sets.

7.4.1. Arbitrary abundances

The **abundances** command can be used to specify the abundances of all elements as a series of numbers. The elements must be in exactly the same order as indicated in Table 9 unless the order is altered with the **elements read** command described on page 56 below. Abundances for all active elements must be specified. Elements can be turned off with the **elements off** command described on page 55 below. The composition can be specified on several lines with **continue** lines following the initial **abundances** line. Abundances of zero are not allowed; Cloudy will stop if they are entered.

N.B. In the following examples the name of an element is written before its abundance. This is only for readability. The code makes no attempt to read the symbols. The numeric abundances *must* appear in the same order expected by the code.

The best way to enter abundances is as *absolute abundances*, as in the following example

```
abundances he =-1 li =-9   be =-11 b  =-9 c  =-4.3 n  =-5 o  =-2.3
continue    f =-7 ne =-1.2 na =-3  mg =-8
continue   al =-8 si =-8   p  =-6  s  =-8 cl =-9   ar =-8 k  =-6
continue   ca =-8 sc =-9   ti =-7  v  =-8 cr =-6.3 mn =-6 fe =-8
continue   co =-9 ni =-8   cu =-7  zn =-7
```

The abundances can also be entered as a set of scale factors indicating the desired abundances relative to the current set absolute abundance. These will be solar by default. The following example doubles the oxygen abundance and lowers the iron abundance

```
abundances he =1 li =1 be =1 b  =1 c  =1 n  =1 o  =2
continue   f  =1 ne =1 na =1 mg =1
continue   al =1 si =1 p  =1 s  =1 cl =1 ar =1 k  =1
continue   ca =1 sc =1 ti =1 v  =1 cr =1 mn =1 fe =0.0000001 //deplete iron
continue   co =1 ni =1 cu =1 zn =1;
```

It is better to specify absolute abundances since the default solar composition changes from time to time.

The code checks the sign of all of the entered abundances to decide which style was entered. The numbers are interpreted as linear scale factors if *all* are positive, and as logs of the abundance relative to hydrogen if *any* are negative.

7.4.2. Setting all at once

If the keyword **_all** appears and exactly one number is entered then all of the elements heavier than hydrogen are given this absolute abundance. The number is the log of the abundance if it is less than or equal to zero and the abundance itself if it is positive. Either of the following commands will give all elements between and

Table 10
Stored Abundance Sets

	Atom	H II Region	Planetary	Nova	Cameron	Primordial	ISM
	key	HII, H II	PLANetary	NOVA	CAMEron	PRIMordial	_ISM
2	He	0.095	0.10	0.098	0.0677	0.072	0.098
3	Li	5.4(-11)	1.0(-20)	2.05(-9)	2.20(-9)	1(-10)	5.4(-11)
4	Be	1.0(-20)	1.0(-20)	2.62(-11)	4.50(-11)	1(-16)	1.0(-20)
5	B	8.9(-11)	1.0(-20)	7.60(-10)	3.40e-10	-	8.9(-11)
6	C	3.0(-4)	7.8(-4)	9.40(-3)	4.22(-4)	-	2.51(-4)
7	N	7.0(-5)	1.8(-4)	9.80(-3)	8.72(-5)	-	7.94(-5)
8	O	4.0(-4)	4.4(-4)	1.70(-2)	6.93(-4)	-	3.19(-4)
9	F	1.0(-20)	3.0(-7)	3.02(-8)	2.90(-8)	-	1.0(-20)
10	Ne	6.0(-5)	1.1(-4)	2.03(-3)	9.77(-5)	-	1.23(-4)
11	Na	3.0(-7)	1.9(-6)	2.06(-6)	2.25(-6)	-	3.16(-7)
12	Mg	3.0(-6)	1.6(-6)	3.80(-5)	3.98(-5)	-	1.26(-5)
13	Al	2.0(-7)	2.7(-7)	2.95(-6)	3.20(-6)	-	7.94(-8)
14	Si	4.0(-6)	1.0(-5)	3.55(-5)	3.76(-5)	-	3.16(-6)
15	P	1.6(-7)	2.0(-7)	3.73(-7)	3.72(-7)	-	1.6(-7)
16	S	1.0(-5)	1.0(-5)	1.62(-5)	1.88(-5)	-	3.24(-5)
17	Cl	1.0(-7)	1.7(-7)	1.88(-7)	1.78(-7)	-	1.0(-7)
18	Ar	3.0(-6)	2.7(-6)	3.63(-6)	3.99(-6)	-	2.82(-6)
19	K	1.1(-8)	1.2(-7)	1.35(-7)	1.35(-7)	-	1.1(-8)
20	Ca	2.0(-8)	1.2(-8)	2.29(-6)	2.35(-6)	-	4.1(-10)
21	Sc	1.0(-20)	1.0(-20)	1.22(-9)	1.16(-9)	-	1(-20)
22	Ti	5.8(-10)	1.0(-20)	8.60(-8)	9.00(-8)	-	5.8(-10)
23	V	1.0(-10)	1.0(-20)	1.05(-8)	9.50(-9)	-	1.0(-10)
24	Cr	1.0(-8)	1.0(-20)	4.84(-7)	4.80(-7)	-	1.0(-8)
25	Mn	2.3(-8)	1.0(-20)	3.42(-7)	3.50(-7)	-	2.3(-8)
26	Fe	3.0(-6)	5.0(-7)	4.68(-5)	3.38(-5)	-	6.31(-7)
27	Co	1.0(-20)	1.0(-20)	2.24(-9)	8.27(-8)	-	1.0(-9)
28	Ni	1.0(-7)	1.8(-8)	1.76(-6)	1.80(-6)	-	1.82(-8)
29	Cu	1.5(-9)	1.0(-20)	1.87(-8)	2.00(-8)	-	1.5(-9)
30	Zn	2.0(-8)	1.0(-20)	4.52(-8)	4.70(-8)	-	2.0(-8)
	grains?	Orion	AGB	no	no	no	ISM

including helium and zinc an absolute abundance of 10^{-10} by number relative to hydrogen:

```
abundances all -10
abundances all 0.000,000,000,1
```

The **metals** command, described on page 66 below, will set abundances of all elements heavier than helium.

7.4.3. Stored abundance sets

Table 10 lists the abundance sets that are stored as a permanent part of the code. These sets are entered if there are no numbers on the **abundances** command, but a keyword occurs, as in the following examples. The four-character part of the keyword that must be matched for the key to be recognized is capitalized in the second line of the table. The following gives some examples:

```
abundances Cameron
abundances HII region [no grains]
abundances h ii region [no grains]
abundances nova
abundances planetary nebula [no grains]
abundances primordial
```

The assumed abundances are from a variety of sources. Table 10 gives their present values.

`Cameron` These are from Cameron (1982). Note that the helium abundance is *very* low, either it or the Big Bang is wrong.

`nova` These are roughly those derived by Ferland & Shields (1978) for the classical nova V1500 Cygni. Abundances close to solar are assumed for those they did not measure.

`H II region` The H II region abundances are a subjective mean of the Orion Nebula abundances determined by Baldwin et al. (1991), Rubin et al. (1991), and Osterbrock et al. (1992). The grains are the large-R size distribution grains described by Baldwin et al. (1991) but with the physics updated as described by van Hoof et al. (2004). The keywords **`HII region`**, **`H II region`**, or **`Orion`** can be used to obtain this abundance set. Abundances of some rare species were taken from the ISM mix of Savage and Sembach (1996). Abundances entered in the table as "1E-20" are not real values, simply values chosen to be small enough to be of no consequence. I would appreciate learning about better numbers.

`planetary nebula` These abundances are from Aller and Czyzak (1983) and Khromov (1989), with high depletions assumed for elements they do not list. The grains are from unpublished work of Kevin Volk on post-AGB stars. The derived dust to gas ratios of different PNe have a large spread. Evidence summarized by Clegg and Harrington et al. (1989) suggests that some PNs have dust to gas ratios roughly ten times smaller than ISM. However, Mallik and Peimbert (1988) find dust to gas ratios similar to ISM and Borkowski and Harrington (1991) find one object with a dust-to-gas ratio an order of magnitude above ISM. The grain composition of planetary nebulae should be treated on a case by case rather than statistical basis. Abundances entered as "1E-20" are not real values, simply values chosen to be small enough to be of no consequence. I would appreciate learning about better numbers.

`_ISM` The gas-phase abundances are an average from the work of Cowie and Songaila (1986) for the warm and cold phases of the interstellar medium together with numbers from Table 5 for the warm and cool phases towards ξ Oph (Savage and Sembach 1996). The oxygen abundance[13] is from Meyers et al. (1998). The grains are the interstellar medium grains defined by Mathis et al. (1977). The ISM, H II

[13] The ISM O abundance was changed from 5.01 to 3.19 × 10^{-4} in version 95.

region, and Orion abundances are not the same, although one can make the case that they should be.

old solar 84 The composition will be the solar used in versions 84 - 94 of the code. These are defined in Table 9 and were taken from the meteoritic abundances of Grevesse and Anders (1989) with extensions by Grevesse and Noels (1993). All three of the keywords **old solar 84** must appear.

Table 11 Old Solar Composition

				Solar	
1	H	Hydrogen	1	0.00	12.00
2	He	Helium	0.1	-1.00	11.00
3	Li	Lithium	2.04E-09	-8.69	3.31
4	Be	Beryllium	2.63E-11	-10.58	1.42
5	B	Boron	7.59E-10	-9.12	2.88
6	C	Carbon	3.55E-04	-3.45	8.55
7	N	Nitrogen	9.33E-05	-4.03	7.97
8	O	Oxygen	7.41E-04	-3.13	8.87
9	F	Fluorine	3.02E-08	-7.52	4.48
10	Ne	Neon	1.17E-04	-3.93	8.07
11	Na	Sodium	2.06E-06	-5.69	6.31
12	Mg	Magnesium	3.80E-05	-4.42	7.58
13	Al	Aluminium	2.95E-06	-5.53	6.47
14	Si	Silicon	3.55E-05	-4.45	7.55
15	P	Phosphorus	3.73E-07	-6.43	5.57
16	S	Sulphur	1.62E-05	-4.79	7.21
17	Cl	Chlorine	1.88E-07	-6.73	5.27
18	Ar	Argon	3.98E-06	-5.40	6.60
19	K	Potassium	1.35E-07	-6.87	5.13
20	Ca	Calcium	2.29E-06	-5.64	6.36
21	Sc	Scandium	1.58E-09	-8.80	3.20
22	Ti	Titanium	1.10E-07	-6.96	5.04
23	V	Vanadium	1.05E-08	-7.98	4.02
24	Cr	Chromium	4.84E-07	-6.32	5.68
25	Mn	Manganese	3.42E-07	-6.47	5.53
26	Fe	Iron	3.24E-05	-4.49	7.51
27	Co	Cobalt	8.32E-08	-7.08	4.92
28	Ni	Nickel	1.76E-06	-5.75	6.25
29	Cu	Copper	1.87E-08	-7.73	4.27
30	Zn	Zinc	4.52E-08	-7.34	4.66
		grains?	no		

7.4.4. Grains, gas-phase depletions, and quantum heating

Certain elements, especially Si, Ca, Al, Mg, and Fe, are heavily depleted onto grains in the ISM. The abundance sets specified by the **h_ii region**, **_ISM**, or **planetary nebula** keywords will include grains and the gas-phase mixtures given in Table 10. The bottom line of the table list the type of grains that are included by default. These types are defined on page 58 below.

Grains can also be specified separately with the **grains** (page 58 below) command. If you use the **grains** command to specify another type of grains then you should include the keyword **no grains** on the **abundances** line to prevent the default grains from also being used.

If you set the keyword **no grains** to not include the default grains and do not specify another set of grains with the **grains** command then grains will not be included in the calculation but the depleted gas-phase abundances will still be used.[14] This is, of course, not self-consistent.

Quantum heating will be considered for all grain species where it will be important. Quantum heating only affects the Wien tail of the grain thermal-emission spectrum. The **no qheat** option on the **abundances** command will disable quantum heating.

Figure 7 compares the continuum predicted in the test case *grains_qheat*, a part of the code's test suite. Quantum heating is normally included and the **no qheat** option was used to disable it to make this comparison.

[14] In versions 77 and before, the abundances of depleted elements were set to solar values when "no grains" was set.

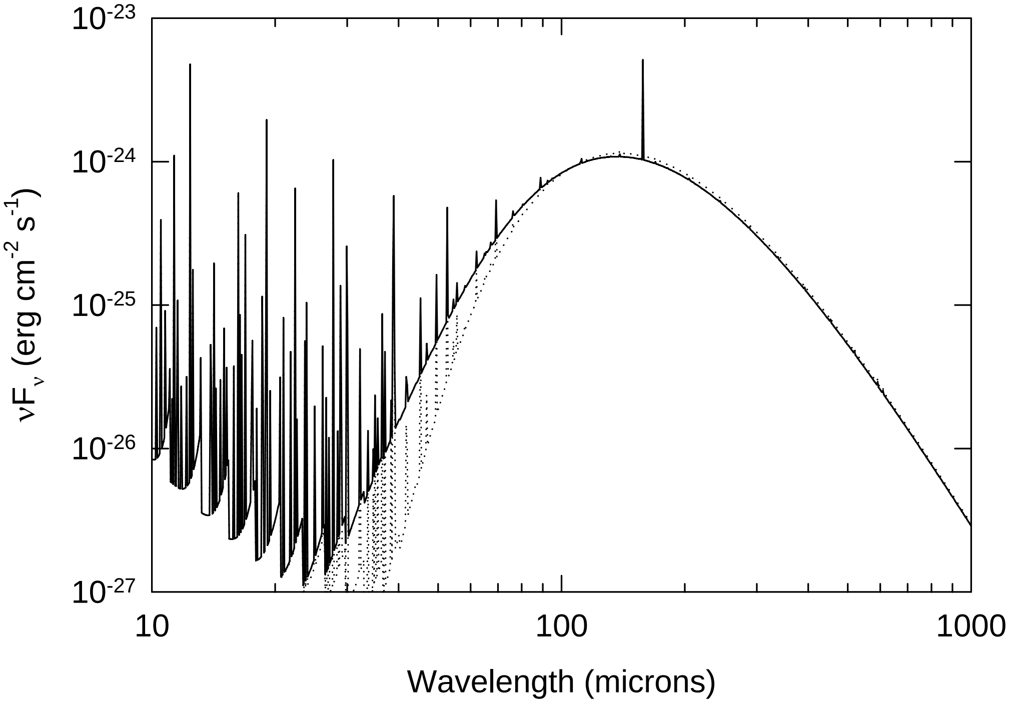


Figure 7 This figure shows the net emission computed by the test case *grains_qheaat*. The solid line includes quantum heating while the dashed line has disabled it.

7.4.5. Interactions between the abundances and grains commands

It is possible to include grain species with both the **`abundances`** command, described here, and with the **`grains`** command, described on page 58 below. For simplicity you should only set the grain abundances only once. If you specify the same grains more than one time you are asking for trouble. The rules for how these commands interact are described on page 60 below.

You should check that you have the expected grain abundances by looking at the list of grain abundances given at the start of the calculation and at the value of $A_V/N_{\rm H}$ given at the end.

7.5. abundances starburst, Z=10

This form of the **`abundances`** command interpolates on Fred Hamann's grid of abundances for an evolving starburst in a massive galactic core. The chemical evolution model is more fully described by Hamann and Ferland (1993). This grid is model M5a of that paper. It uses a star formation rate and infall timescales very close to, but slightly faster than, the "standard" elliptical model (see also Arimoto and Yoshii 1987; Matteucci and Greggio 1986; Matteucci and Tornambe 1987; Bica 1988). Its IMF also has a slope very similar to, but slightly steeper than (x = 1.0 instead of 1.1), that of the standard elliptical model. The main difference is that the IMF has a lower mass cutoff at $M = 2.5\ M_{/}$ instead of $\sim$0.1 $M_{/}$ in the standard models. This allows the gas to reach much higher metallicities before the gas is locked up in low-mass stellar remnants.

The metallicity of the gas relative to solar appears on the line. It is interpreted as the log of the metallicity if it is less than or equal to zero, and the linear metallicity if positive. The keywords **`_log`** or **`linear`** will force the number to be interpreted appropriately. The limits to the range of possible metallicities are $10^{-3}Z_{/}$ and 36 $Z_{/}$.

This command works by generating scale factors that multiply the current standard abundance. This is solar by default. The command does not derive absolute abundances. If you change the abundances with a second **`abundance`** command then the scale factors will multiply those new abundances.

The keyword **`trace`** will print the abundances of all elements as a function of metallicity between the full $10^{-3}Z_{/}$ and 36 $Z_{/}$ limits. The code will then stop.

7.6. element name [scale, abundance, _off, _log, table]

This sets the abundance of a particular element. The command has several keywords that change what the command does. The name of an element as spelled in Table 9 must appear.

7.6.1. element name scale

If the keyword **`scale`** appears then the number on the line is a scale factor multiplying the current abundance of the element. The number is a linear scale factor if it is positive or if the **`linear`** keyword appears and it is the log of the scale factor if the number is negative. If the key **`_log`** appears (note the leading space) then the scale factor is interpreted as a log irregardless of its sign.

7.6.2. element name abundance

If **`abundance`** appears then the number is the absolute abundance of the element by number relative to hydrogen. The number is the log of the abundance unless the **`linear`** keyword appears.

7.6.3. element name ionization

This allows the ionization distribution of an element to be set. Each number is the ionization fraction, $n(A^{+i})/n(A)$, for successive stages of ionization. The code will scan off up to A+1 numbers, where A is the atomic number of the element. If any numbers are negative then all are interpreted as logs of the ionization fraction. If there are fewer than A+1 numbers then the missing stages of ionization are assumed to have zero abundance.

This command does not confirm that the sum of the ionization fractions is unity. The abundance of each stage of ionization is set to the product of the ionization fraction times the total gas-phase abundance. If the fractions do not add up to unity the effect will be to change the total abundance of the element.

This command does not specify its chemical state. The H_2 fraction can be set with the **`set H2`** command described on page 211 below. Chemistry is disabled if you set the ionization distribution of an element that is part of the chemical network. It will not be possible to obtain a chemical solution if the abundances of the atom and ions cannot respond to changes in the chemistry.

All of this is unphysical and is only intended as a way to test the code.

7.6.4. *element name off*

If the keyword _**off** appears (note the leading space) then the element is not included in the calculation. The ionization equilibrium, opacity, and cooling due to the element will not be computed. The abundance must still be specified when the **abundances** command (page 49 above) is used unless the element is excluded with the **elements read** command (page 49 below).

The keyword _**on**_ will include an element that was previously turned off in the same input stream.

You can save computer time if you turn an element off. This is especially true for third- and fourth-row elements. These take longer to compute because of the large number of inner-shell electrons. They often have negligible effects on the thermal and ionization structure because of their low abundances.

Memory for the species that are present is dynamically allocated when the code starts. When the code is used to compute a large grid of models it is not possible to turn on an element that was turned off for the first model since the needed memory does not exist. You can turn off an element in later models since the element is simply not computed. In later calculations in a grid the code will ignore any attempt to turn on an element that was initially turned off.

The chemical solution may become destabilized if an element that forms molecules is turned off. Do not turn off elements that are part of the chemistry if the calculation extends into a PDR or molecular cloud. The code will generate a warning if this is done.

Turning off an element with this command has many other side effects. For instance, the following input stream would produce unexpected results:

```
element zinc ionization -3 0 -4
init “ism.ini”
element zinc on
```

because the *ism.ini* file turns off zinc. This destroys the memory of the **element zinc ionization** command, which sets the ionization of the element. So, when the element is turned back on with the **element zinc on** command the ionization will be determined self consistently rather than set to the constant values.

7.6.5. element limit off -12

Elements with abundances that are smaller than the number on the line will be ignored. The number is the log of the limiting abundance by number relative to hydrogen. This is an easy way to turn off elements that have trivial abundances. The adjoining table lists the elements in terms of decreasing abundance. The command

```
elements limit off -7
```

would cause all elements at Cobalt and above in the table to be turned off.

A	symbol	name	Log n/H
4	Be	Beryllium	-10.58
5	B	Boron	-9.21
21	Sc	Scandium	-8.83
3	Li	Lithium	-8.69
23	V	Vanadium	-8.00
29	Cu	Copper	-7.79
9	F	Fluorine	-7.52
30	Zn	Zinc	-7.40
27	Co	Cobalt	-7.08
22	Ti	Titanium	-6.98
19	K	Potassium	-6.88
17	Cl	Chlorine	-6.72
25	Mn	Manganese	-6.54
15	P	Phosphorus	-6.50
24	Cr	Chromium	-6.33
28	Ni	Nickel	-5.75
11	Na	Sodium	-5.67
20	Ca	Calcium	-5.64
18	Ar	Argon	-5.60
13	Al	Aluminium	-5.53
16	S	Sulphur	-4.74
26	Fe	Iron	-4.55
12	Mg	Magnesium	-4.46
14	Si	Silicon	-4.46
7	N	Nitrogen	-4.07
10	Ne	Neon	-4.00
6	C	Carbon	-3.61
8	O	Oxygen	-3.31
2	He	Helium	-1.00
1	H	Hydrogen	0.00

7.6.6. elements read

Normally Cloudy expects the abundances entered with the **abundances** command to occur in exactly the same order as the atomic numbers of the elements. These begin with helium and include all elements through zinc. The **elements read** command makes it possible to change this order or to leave certain elements out entirely. The command begins with the line **elements read**, follows with a list of elements, and ends with a line beginning with the keyword **end**.

This order will be used for all **abundances** commands that follow this command. If an element does not occur in the list then its value cannot be set by an **abundances** command. This does not turn an element off – this is done with the **element name off** command, described on page 55 above.

The following example shows an input stream that changes the **abundances** command so that it behaves more like version 84 of the code. Only the elements in the list were present in that version. The **elements read** command sets the elements that will be entered then the missing elements are turned off with the **element off** command.

```
elements read
helium
carbon
nitrogen
oxygen
neon
sodium
magnesium
aluminum
silicon
sulphur
```

```
argon
calcium
iron
nickel
end of elements
c
element Lithium off
element Beryllium off
element Boron  off
element Fluorine  off
element Phosphor off
element Chlorine off
element Potassium off
element Scandium  off
element Titanium off
element Vanadium off
element Chromium off
element Manganese off
element Cobalt off
element Copper off
element Zinc  off
```

In summary: Turning an element off with the **element off** command does not remove that element from the list of abundances entered with the **abundances** command. Leaving an element out of this list with the **elements read** command does not turn off that element.

7.6.7. element name table

If the keyword **table** appears on the **elements** command then the code will read in a list of position-dependent abundances for a particular element. This might, for instance, be used to model variable depletions. The following is an example.

```
element carbon table depth
-30 -4
3 -4
5 -3
7 -2
9 -1
end of table
```

The first number on each line is the log of the radius (the default) or depth (if the keyword **depth** also appears on the **element** line). Depth and radius are defined on page 8 above. The second number is the log of the abundance of the element at that point, by number relative to hydrogen. The table ends with a line starting with the keyword **end**. Up to 500 pairs may be entered. This command always specifies the absolute abundance and not the scale factor.

The chemical composition printed at the start of the calculation is always the composition at the illuminated face of the cloud. If the table gives composition as a function of radius then the composition will be evaluated at the inner radius of the cloud. If the table gives the composition as a function of depth then the composition will be evaluated as a depth of 10^{-30} cm. The table must extend to this depth as in the example above.

7.7. fluctuations abundances, period, max, min, phase

This makes the metallicity vary with radius as a sine wave. This is designed to investigate the effects of chemical inhomogeneities upon the emission-line spectrum and was implemented to search for solutions to the t^2 problem (Kingdon & Ferland 1995).

The first number is the log of the period P of the sine wave in centimeters. The second two numbers are the logs of the largest and smallest metallicities over the sine wave and have the same effect as the metals scaling factor entered with the **`metals`** command (page 66 below).

The **`fluctuations`** command is more fully described in the description of the density version on page 71 below.

7.8. grains

This command controls how grains are included in the calculation. They are not included by default. They are included in the compositions set by some abundances commands (see page 49 above). Grain physics was developed in collaboration with Peter van Hoof, Peter G. Martin, and Joe Weingartner, and Peter van Hoof did the majority of the coding. Reviews are given by Spitzer (1948; 1978), and Martin (1979). Baldwin et al. (1991), Weingartner & Draine (2001b), van Hoof et al. (2004) and Weingartner et al. (2006) describe the theory incorporated in the code.

The **`punch grain`** commands, described on page 153 below, produce output giving details about the grains. Some details of the grain physics can be adjusted with the **`no grain`** family of commands, described on page 202 below.

7.8.1. Using the built-in grain types

The grain types summarized in Table 12 are included in the code's data files. The table gives the grain material, its size distribution, and the name of the grain opacity file that it uses. In most cases these will be sufficient – nothing more needs to be done to set up the grains.

Grains are composed of elements that are depleted from the gas phase. It would be inconsistent to assume solar abundances for all elements and also include grains. In reality certain elements, especially Ca, Al, Ti, and Fe, are missing from the gas phase and are believed to be present as grains. The **`metals deplete`** command (see page 66 below) can be used to deplete elements that are included in grains.

Several of the standard abundance sets that are used with the **`abundances`** command (page 49 above) include grains. The elements which make up the grains are depleted from the gas phase in these abundance sets. Elements are not depleted in sets that do not include grains by default.

`grains _ISM` specifies grains with a size distribution and abundance appropriate for the ISM of our galaxy. This includes both a graphitic and silicate component and generally reproduces the observed overall extinction properties for a ratio of extinction per reddening of $R_V \equiv Av/E(B\text{-}V) = 3.1$. This is the default and will be used if no keywords occur on the **`grains`** command. If either keyword **`graphite`** or **`silicate`** also appears then only that grain type is included. Both species are included if neither keyword appears.

grains Orion specifies graphitic and silicate grains with a size distribution and abundance appropriate for those along the line of sight to the Trapezium stars in Orion. The Orion size distribution is deficient in small particles and so produces the relatively grey extinction observed in Orion (Baldwin et al. 1991). If either keyword **graphite** or **silicate** appears then only that grain type is included. Both species are included if neither keyword appears.

grains PAH turns on PAHs. See page 60 below for more details.

grain abundances An optional scale factor on the command line changes the grain abundance relative to its default value. If the keyword **_log** appears or if the number is less than or equal to zero then the number is the log of the scale factor. It is the linear factor if the keyword **linear** appears or if no keyword appears and the number is positive.

It is also possible to change the abundances of the grains with the **metals grains** command (see page 66 below). The **metals** command scales the abundances of all elements more massive than helium by a scale factor. If the keyword **grains** occurs then the grain abundance will also be scaled up or down. This would keep the grains to metals abundance ratio constant.

The following example uses ISM gas phase abundances, Orion silicates with dust to gas ratio twice the default value, and ISM graphite with default ISM abundances.

Table 12 Standard Grain Types

Keyword	Filename	Type	Size distribution
	graphite_0m010.opc	Graphite	Single 0.01 μm
	graphite_0m100.opc	Graphite	Single 0.1 μm
	graphite_1m000.opc	Graphite	Single 1 μm
ISM single graphite	*graphite_ism_01.opc*	Graphite	Unresolved ISM
ISM graphite	*graphite_ism_10.opc*	Graphite	ISM, 10 bins
Orion single graphite	*graphite_orion_01.opc*	Graphite	Unresolved Orion
Orion graphite	*graphite_orion_10.opc*	Graphite	Orion, 10 bins
grey	*grey_ism_01.opc*	Grey	Unresolved ISM
grey	*grey_ism_10.opc*	Grey	ISM, 10 bins
	pah1_0n341.opc	PAH	0.00034 μm
	pah1_0n682.opc	PAH	0.00068 μm
PAH single	*pah1_ab08_01.opc*	PAH	Unresolved AB08
PAH	*pah1_ab08_10.opc*	PAH	AB08, 10 bins
	silicate_0m010.opc	Silicate	Single 0.01 μm
	silicate_0m100.opc	Silicate	Single 0.1 μm
	silicate_1m000.opc	Silicate	Single 1 μm
ISM single silicate	*silicate_ism_01.opc*	Silicate	Unresolved ISM
ISM silicate	*silicate_ism_10.opc*	Silicate	ISM, 10 bins
Orion single silicate	*silicate_orion_01.opc*	Silicate	Unresolved Orion
Orion silicate	*silicate_orion_10.opc*	Silicate	Orion, 10 bins

```
// use ISM abundances but DO NOT include ISM default grains
abundances ISM no grains
// Orion silicate with twice the Orion abundance
grains Orion silicate 2
// ism graphite with ISM dust to gas ratio
grains ISM graphite
```

The default H II region grain abundances are close to the ISM value. Planetary nebula grain abundances are quite uncertain. Clegg and Harrington (1989) find dust-to-gas ratios below the ISM value, while Borkowski and Harrington (1991) find a dust-to-gas ratio an order of magnitude above ISM in a hydrogen-deficient planetary nebula. Mallik and Peimbert (1988) find dust-to-gas ratios roughly equal to the ISM in a sample of PNs. Stasinska & Szczerba (1999) discuss properties of a sample of PNe. In view of this scatter the grain abundance of PNe should probably be treated as a free parameter.

Size resolved or averaged grains Grains in the ISM have a broad range of sizes, often described by a power-law distribution (Mathis, Rumpl & Nordsieck 1977). By default the grains will be resolved into ten size bins. If the keyword **single** appears then the grains will have properties determined by averaging over the entire size range. If the keyword **distribution** appears then the code will resolve the size distribution. This is the default and will be used if no keyword appears. The **single** option may save some machine time but will give a less realistic representation of the grain physics. This is because many grain properties such as temperature and charge depend strongly on the size. In particular, the photoelectric heating of the gas can be underestimated if the single mean grain is used.

7.8.2. Interactions between abundances and grains commands

Be careful when specifying grains with more than one **grains** command or with both the **abundances** and **grains** commands. The order in which the commands appear in the input stream does make a difference. These commands have the following precedence:

- An **abundances** command will override all grains set with a previous **abundances** command. So with the following pair

```
abundances ism
abundances old solar 84
```

ISM grains stay in place!

```
abundances ism
abundances orion
```

only Orion grains will be included

- An **abundances** command will NOT override any grains set with a previous **grains** command. It will not add any grains either. Instead it will implicitly behave as if the option **no grains** was given on the **abundances** command.

```
grains orion
abundances ism
```

only Orion grains are included

- A **grains** command given after an **abundances** command or another **grains** command will add to those already included, even if it would cause the same set of grains to be included twice. A warning will be printed if the latter occurs. For instance, the following would add the ISM grains twice and generate a warning;

```
abundances ism
grains ism
```

- An **abundance** command that does not set any grains will not override any grains set with a previous **abundances** command.

The following would result in the Orion gas-phase composition but ISM grains

```
abundances Orion no grains
grains ism
```

The following will use ISM grains and Orion abundances, but will not include Orion grains since the **abundances** command comes after the **grains** command;

```
grains ism
abundances Orion
```

The order is swapped in the following. This results in Orion gas-phase abundances and both ISM and Orion grains

```
abundances Orion
grains ism
```

To avoid confusion it is best to only specify grains with only the **abundances** command or by including the **no grains** option on the **abundances** command and then including explicit **grains** commands. In any case, be sure to check the resulting output to verify that things are set properly.

7.8.3. Creating your own grain types

New types of grains may be introduced by first generating data files that specify the size distribution and refractive indices for the full energy range considered by the code. These are then converted to opacities with the **compile grains** command. The process is described further where the **compile grains** command is discussed (page 193 below). The result is a new *opc* file.

The code will read an opacity file whenever a double quote (") occurs anywhere on the command line. If a double quote is found then the code will look for the name between a pair of quotes, as in "**special.opc**", and will stop if the file cannot be found or if the second quote is missing. If the file exists then this grain species will be included. So don't place a quote on the **grains** command unless there is a pair of quotes surrounding a filename since the code will stop. The contents of that file will determine whether the calculations are size-resolved or not, irrespective of the keywords **distribution** or **single**.

7.8.4. PAHs

PAH's are not included by default but are added with the **grains PAH** command. A detailed treatment of the physics of PAH's is implemented, including photoelectric heating and collisional processes as discussed by Weingartner & Draine (2001), and stochastic heating effects following Guhathakurta & Draine (1989). A power-law distribution of PAH sizes with 10 size bins (Abel et al 2008, hereafter AB08), and two single-sized PAH's, are included in the downloaded data files. AB08 is the default and will be used if no further options occur on the command line. If the keyword **single** also appears then an unresolved size distribution with their mean properties is used.

The PAH opacity functions were derived by Kevin Volk from a variety of sources. The original opacity function is from Desert, Boulanger, & Puget (1990) and Schutte, Tielens, & Allamandolla (1993). Kevin adapted the opacities from these papers to agree with the infrared plateaus seen in the Orion Bar (Bergmann et al. 1988). The optical/far-UV opacity values have a gradual change to atomic cross sections so that you get the correct X-ray cross sections.

The command **grains PAH C15**will include a single small PAH with 15 carbon atoms per molecule, with an abundance relative to hydrogen of $n(\mathrm{PAH})/n(\mathrm{H}_{tot}) = 1.986\times10^{-7}$, corresponding to $n(\mathrm{C})/n(\mathrm{H}_{tot}) = 2.979\times10^{-6}$. The command **grains PAH C120** will include a large PAH with 120 carbon atoms per molecule and an abundance relative to hydrogen of $n(\mathrm{PAH})/n(\mathrm{H}_{tot}) = 2.483\times10^{-8}$, also corresponding to $n(\mathrm{C})/n(\mathrm{H}_{tot}) = 2.979\times10^{-6}$.

PAHs appear to exist mainly at the interface between the H^+ region and the molecular clouds. Apparently PAHs are destroyed in ionized gas (Sellgren et al. 1990, AGN3 section 8.5) by ionizing photons and by collisions with ions (mainly H^+) and are depleted into larger grains in molecular regions. The code assumes that the PAH abundance scales with the ratio $n(\mathrm{H}^0)/n(\mathrm{H})$. This produces very few grains in ionized and fully molecular gas, but the PAHs will have their default abundance when the gas is atomic. This is consistent with Sellgren's observations of the Orion Bar.

The **set PAH** command (page 215 below) makes it possible to specify several other laws describing how PAH abundances depend on physical conditions. Note that if PAHs are present in predominantly molecular gas then they will soak up nearly all of the free electrons. This is not observed and may destabilize the chemistry network.

7.8.5. Variable grain abundances

The **function** option on the **grains** command makes it possible to vary the abundance of any grain species across a cloud. (The **abundances** command does not have the **function** option.) This option works by setting the local abundance of a grain species to the product of the intrinsic abundance and the value returned by the function *GrnVryDpth*. That routine can be modified by the user to specify a scale factor that might depend on other physical conditions or location. All the other multipliers for the grain abundance are still in effect when the keyword **function** is used. This means that the abundance multiplier supplied with the **grains** command is also included, as well as the factor supplied in the **metals grains** command (see page 66 below). So the abundance of the grain is given by the default abundance multiplied with the two numbers mentioned here times whatever *GrnVryDpth* returns.

If the **grains** command sets the abundance of a single grain species then the **function** option will only apply to that particular species. If the option occurs on a **grains** command that specifies more than one species of grains (as in the **ISM** keyword) then all species enabled by that command are affected. This is probably unphysical since small grains are easier to destroy than large grains. However, it is possible to define a different behavior of the grain abundance in routine ***GrnVryDpth*** for each individual grain size bin.

The code does not attempt to conserve the mass of the grain constituents. The gas-phase abundances are not automatically changed where the grains are changed. This can be done by entering abundances with a depth-dependent table of abundances using the **elements read** command (see page 56 above).

7.8.6. Line intensities with grains.

Two sets of line intensities, the intrinsic and emergent spectra, are predicted. These differ because the observed spectrum of an emission-line region containing dust depends on the geometry and the viewing angle.

The intrinsic spectrum: This is the spectrum produced within the cloud and does not include effects of dust that lies outside the line-forming region. Photon destruction by all background opacity sources (including grains) is fully treated (i.e., Hummer 1968), and the predicted intrinsic intensities always includes this destruction. These intensities *do not* include the reddening effects of any grains or other opacity sources that lie outside the line-forming region.

The emergent spectrum: This would be the spectrum if the geometry were observed from the illuminated face of the cloud. It assumes that the ionized gas has a large molecular cloud behind the shielded face of the ionized gas. The emergent line intensities include contributions from absorption by grains, and reflection off the molecular cloud.

The effects of grains external to the emission-line region are very geometry dependent. One approach is to correct the observed spectrum for reddening to obtain an intrinsic spectrum, and to then compare this intrinsic spectrum with that computed by the code.

These issues are discussed further in the section *Line intensities in a dusty open geometry*, in the chapter *Observed Quantities*, in Part 3 of HAZY.

7.8.7. Extinction for point and extended sources

Grain extinction is given by the cross section [cm^2] per H nucleon: $\sigma = \kappa / n\left(\mathrm{H}\right)$, where κ [cm^{-1}] is the opacity due to grains and n(H) [cm^{-3}] is the local density of H in all forms. The opacity includes both absorption and scattering. The scattering opacity depends on the geometry of the absorbing cloud, as described next and in AGN3 section 7.3.

Light scattering off grains is not isotropic. The angular dependence is often approximated by the Henyey-Greenstein function. The scattering theory predicts the fraction of scatterings, given by the grain asymmetry factor *g*, that are “forward scattering”, that is, change the direction of the scattered photon by less than 90 degrees (i.e. into the forward 2π sr). The asymmetry parameter *g* is defined as the average value of cos(θ), where θ is the angle between incident and scattered photon. So for isotropic scattering *g* = 0, while for strongly forward scattering, *g* will be close to 1.

Rather than the total scattering cross section σ_s, an effective scattering cross section $\sigma_{scat} = \sigma_s (1\text{-}g)$ contributes to extinction for extended sources. This discounts light scattered into the forward 2π sr. The asymmetry parameter *g* approaches unity at high energies, so that σ_{scat} becomes much less than σ_{abs}. For an extended source such as a diffuse cloud the loss of photons by small-angle scattering will be compensated by a similar gain of photons from rays that are nearly parallel, so that total opacity is $\sigma_{abs} + \sigma_s(1\text{-}g)$. This is referred to as extended source extinction and would apply to a resolved H II region like the Orion Nebula.

For a point source such as a star even a small deflection of starlight by forward scattering removes light from the ray and so counts as extinction. In this case the total grain opacity is simply $\sigma_{abs} + \sigma_s$. This is referred to as the point source extinction and is the quantity measured in extinction studies of stars.

The code keeps track of both measures of extinction since a beam of light passing through an H II region is attenuated by the extended extinction while the observational stellar literature will quote a point source extinction.

7.8.8. Grains-related commands

A group of **`no grain`** commands, which turn off various physical processes, is described on page 202 below.

There are several **`punch`** commands that will output predicted properties of the grains. The **`punch grains`** command (page 153 below) will give some additional information about the grain properties. The files produced by the **`punch continuum`** (page 143 below) and **`punch spectrum`** (page 171 below) commands will include the infrared continuum emitted by the gas and grains.

`grain no heating` or **`no cooling`** The keyword **`no heating`** on the **`grains`** command will turn off heating of the gas by grain photoelectric emissions. The keyword **`no cooling`** will turn off all forms of cooling of the gas by collisions with the grains. Either violates energy conservation, of course.

`grains no reevaluate` The **`no reevaluate`** option on the **`grains`** command will speed up a calculation by not continuously reevaluating grain quantities. Roughly a 30% speedup can be achieved. This is potentially dangerous and can destabilize a solution and/or lead to wrong results. It should be used under certain experimental circumstances and not in a true simulation of a cloud.

`set nchrg` The grain charge distribution is resolved into the number of discrete integral charge states set by the **`set nchrg`** command. The default is two charge states. The population of each of charge state is determined self-consistently by solving the grain ionization-recombination balance equations as described in van Hoof et al. (2004).

Forcing quantum heating on or off By default, quantum (also called “stochastic” or “single-photon”) heating is included for size-resolved species when it is significant. Guhathakurta and Draine (1989) describe the formalism used here. The method was originally implemented by Kevin Volk and subsequently revised and generalized by Peter van Hoof. This is considered for all species except for the unresolved size distributions. To save time, quantum heating is only treated when the grain cooling time is sufficiently short compared with the time between heating events. Quantum heating is considered for a given size bin if the ratio of the volume of the largest and the smallest grain in that particular bin is less than 100. This means that quantum heating is considered for all of our resolved distributions, as well as all single-sized grains, but not for unresolved distributions (except the unresolved AB08 distribution, where it ***is*** used by default).

In the zone printout an asterisk will appear next to the name of a grain if quantum heating is important.

The keyword **`qheat`** will force quantum heating to always be considered for species where it is important. This is the default for all resolved size distributions this keyword is not needed. The keyword **`no qheat`** will disable quantum heating for an individual **`grains`** command. Grain species with quantum heating enabled and disabled can be mixed.

Quantum heating can be turned off for all species with the **`no grain qheat`** command described on page 203 below.

7.8.9. Effects of grains

Grains have several effects on interstellar gas (see AGN3, Chapter 7). Refractory elements are depleted from the gas phase, thus removing coolants from the gas (Kingdon, Ferland, & Feibelman &1995). Grains absorb the incident continuum and reradiate an infrared continuum (Bottorff et al. 1998). Higher-energy photons ionize the grains, establishing a net charge, and so affect the charge balance of the gas (Baldwin et al. 1991). Photoejection of electrons following absorption of a UV photon heats the gas. Grains surfaces are sites of important chemical reactions, atomic/ion charge transfer, and molecular freeze-out when temperatures become low. Grains are a net sink of free electrons in fully molecular regions – this greatly influences PDR models. Several processes partially couple the temperatures of the gas and dust (van Hoof et al. 2004).

The heating and cooling of the grains and gas are done self-consistently. Grains are heated by direct absorption of the incident continuum, by the line and continuum emission within the cloud, and by gas collisions. Grains cool by collisions with the gas, the thermionic effect, and by radiation. The balance between heating and cooling establishes the temperature for each grain size and type. Grains affect the gas temperature by heating, mainly by the grain photoelectric effect and the thermionic effect, and by cooling, mainly by free-particle capture onto the grain surface.

7.9. metals 0.05 [_log, linear, grains; deplete]

This command multiplies the abundances of the entire mixture of metals (elements heavier than helium) by the scale factor entered on the line. This is useful when the effects of global enrichments or depletions of the elements are to be investigated. If the number is less than or equal to zero it is assumed to be the log of the scale factor and the linear scale factor if it is positive. The **linear** and **_log** keywords force that interpretation of the number.

Combinations such as

```
abundances planetary nebula
metals 3
```

or

```
metals 3
abundances planetary nebula
```

would multiply the planetary nebula gas-phase abundances by three,[15] while

```
metals -10
```

would multiply the default solar mixture by 10^{-10}.

7.9.1. Scaling grains and metals together

It seems likely that the grain to hydrogen ratio scales with the total gas-phase metallicity. The optional keyword **grains** on the **metals** command causes the grain abundance to also be scaled by the factor on the line. The basic assumption is that the grain to metals ratio does not depend on metallicity while the grain to gas (hydrogen) ratio depends linearly on the metallicity. It is still necessary to include grains with either the **grains** command or by specifying a chemical composition that contains grains (with the **abundances** command). The scale factor that appears on the **metals** command will further multiply the grain abundance specified on the **grains** command. That is, the combination

```
grains .5
metals and grains .5
```

(in any order) will result in a grain abundance that is a quarter of the default and a metallicity that is half of solar.

In the following example the ISM gas phase *and* grain abundances are each increased by a factor of two over their default values;

```
abundances ISM
metals and grains 2
```

7.9.2. metals deplete - gas-phase depletion factors

It is possible to alter an existing set of abundances by depletion onto grains. In the ISM the observed depletion is a function of the gas density (Spitzer 1985 models this), so there is not really a universal depletion pattern. A set of scale factors that are roughly those appropriate for relatively dense ISM gas (~1 cm^{-3}) is built into the

[15] Limits to the ordering of the **abundances** and **metals** commands existed before version 72 but have been lifted.

code. Table 13 lists the depletions that will be assumed if the keyword **deplete** occurs on the **metals** command, but no numbers are on the line. These are loosely based on the depletions listed by Jenkins (1987) and Cowie and Songaila (1986). This table is obviously incomplete and I would appreciate learning of better references.

This command can be combined with commands that specify abundances, and the **grains** command to specify an arbitrary set of grain and gas-phase abundances. Specifying grains by themselves (with the **grains** command) does not change the gas-phase abundances, which is not self-consistent. The code will complain if you do this, but still perform the simulation.

The following is an example of using the nova abundance mixture, depleting it with this command, and then setting ISM grains.

```
abundances nova
metals deplete
grains
```

These commands do not attempt to conserve mass. In particular, the grain mass will be less than the mass of depleted heavy elements because the nova mixture has enhanced CNO, while the ISM grains have only a corresponding solar depletion of missing material (see, however, Snow & Witt 1996, who show that even this is not true).

Note that Tables 13, 10, and 9 are not self-consistent since they come from different sources.

Table 13
Depletions

	Depl	Reference
He	1.00	noble gas
Li	0.16	White 1986
Be	0.6	York et al 1982
B	0.13	Federman et al 1993
C	0.4	
N	1.	
O	0.6	
F	0.3	Snow and York 1981
Ne	1.0	noble gas
Na	0.2	
Mg	0.2	
Al	0.01	
Si	0.03	
P	0.25	Cardelli et al 1991
S	1.0	
Cl	0.4	
Ar	1.0	noble gas
K	0.3	Chaffee& White 1982
Ca	1(-4)	
Sc	5(-3)	Snow, Dodger 1980
Ti	8(-3)	Crinklaw et al 1994
V	6(-3)	Cardelli 1994
Cr	6(-3)	Cardelli et al 1991
Mn	5(-2)	Cardelli et al 1991
Fe	1(-2)	
Co	1(-2)	
Ni	1(-2)	
Cu	0.1	Cardelli et al 1991
Zn	0.25	Cardelli et al 1991

8. DENSITY LAWS

8.1. Overview

Hydrogen plays a fundamental role in any astrophysical plasma because of its large abundance. As a result the hydrogen density [cm^{-3}] is a fundamental parameter. Commands that specify how the hydrogen density is set, and how it changes with radius or depth, are described in this section. Constant density is the default. In this case the total hydrogen density (the sum of the protons in atomic, ionic, and molecular form, given by the command **hden** described on page 72 below) is kept constant. Many other density or pressure distributions can also be computed.

A cloud can be isobaric, maintain constant pressure, if the timescale for changes, for instance in the continuum source or the cooling time, is short compared with the dynamical or sound-crossing time t_d

$$t_d = \frac{\Delta r}{c_s} \quad [\mathrm{s}] \tag{26}$$

where Δr is the cloud thickness and c_s is the sound speed (AGN3 eq 6.25)

$$c_s = \left(\frac{\gamma k T_0}{\mu_0 m_\mathrm{H}} \right)^{\frac{1}{2}} \quad [\mathrm{cm\ s^{-1}}]. \tag{27}$$

8.2. constant density, pressure, gas pressure

This command specifies how the density changes across the cloud. The **hden** command usually specifies the initial hydrogen density. Several commands determine how the density changes with radius. These are described next.

8.2.1. constant density

This is the default. The hydrogen density, the sum

$$n(\mathrm{H}) = n\left(\mathrm{H}^0\right) + n\left(\mathrm{H}^+\right) + 2n(\mathrm{H}_2) + \sum_{other} n\left(\mathrm{H}_{other}\right) \quad [\mathrm{cm^{-3}}] \tag{28}$$

is kept constant. This is not quite an isochoric density law because the total particle density is not constant —the electron and molecular fractions can vary with depth. I prefer this type of model because the homology relations with the ionization parameter (Davidson 1977) are preserved. The hydrogen nucleon density is set with the **hden** command (page 72 below).

8.2.2. constant gas pressure [index =-1.1]

An isobaric density law is specified with this command. The gas pressure

$$P_{gas} = n_{tot} k T_e \quad [\mathrm{dyne\ cm^{-2}}] \tag{29}$$

where n_{tot} is the total particle density [cm^{-3}], is kept constant. The optional index α can be any value, positive or negative, and will force the pressure to change as a power-law of the radius;

$$P_{gas}(r) = P_o \left(\frac{r}{r_o} \right)^{\alpha} \quad \text{[dyne cm}^{-2}\text{]} \qquad (30)$$

where P_o is the pressure at the illuminated face of the cloud.

8.2.3. constant pressure [no continuum, no abort]

This holds the total pressure constant. This includes ram, magnetic, turbulent, particle, and radiation pressure. The equation of state is given by

$$\begin{aligned} P_{tot}(r) &= P_{tot}(r_o) + \int a_{rad}\, \rho\, dr \\ &= P_{gas} + P_{lines} + P_{continuum} + P_{ram} + P_{turb} + P_{magnetic} \end{aligned} \quad \text{[dyne cm}^{-2}\text{]} \qquad (31)$$

where a_{rad} is the radiative acceleration [cm s^{-2}] due to the attenuated incident continuum and ρ is the density (gm cm^{-3}).

The terms are the following: $P_{gas} = n_{tot} k T_e$ is the thermal gas pressure. The outward force due to the attenuation of the incident radiation field is given by the integral and referred to as $P_{continuum}$. The **no continuum** option will turn this off. The ram pressure is P_{ram} = ρu_{wind}^2 where u_{wind} is the flow velocity. This is only present for a wind geometry (see page 115 below). The turbulent pressure is $P_{turb} = \rho\, u_{turb}^2 / 2$ where u_{turb} is the turbulent velocity as set with the **turbulence** command (page 100 below). The magnetic pressure is $P_{mag} = B^2 / 8\pi$ where the magnetic field B is set with the **magnetic field** command (page 109 below). Both magnetic and turbulent pressures are zero by default since turbulence and magnetic fields are not included by default. They must be independently specified. If either turbulent or magnetic pressure dominates the total pressure then the density will be nearly constant.

P_{lines} is the nearly isotropic radiation pressure due to trapped emission lines (Ferland & Elitzur 1984, and Elitzur & Ferland 1986). Cloudy will stop if the internal line radiation pressure builds up to more than half of the total pressure since such clouds would be unstable unless they are self-gravitating (Elitzur and Ferland 1986). It is necessary to do at least a second iteration when radiation pressure is important since the total line optical depths must be known to compute line widths and level populations reliably. If more than one iteration is done then the radiation pressure will not be allowed to exceed the gas pressure on any except the last iteration. If the option **no abort** appears on the command line the code will never stop because of excessive radiation pressure. The radiation pressure is still computed and the simulation will probably become unstable when $P_{lines} > P_{gas}$.

8.2.4. constant pressure set 6.5

The **_set** option specifies the initial pressure. A number, the log of the pressure in ISM nT units (K cm^{-3}), must appear.

An initial gas density must still be specified with one of the commands in this Chapter. This command works by first solving for the equilibrium temperature at the density that was specified. The density is then changed, using a Newton-method solver, to have the pressure match that specified. The solver will raise or lower the density assuming that pressure and density are directly related to one another.

There are possible ambiguities in this solution since the same pressure can sometimes be achieved with more than one density. This is the well-known three-phase stability phenomenon (Field et al 1969).

8.3. dlaw [options]

An arbitrary density law, specified by the user, will be used. There are two forms of this command. It is possible to either edit the source to create a new routine that calculates the density at an arbitrary depth or to interpolate on a table of points.

If the density or density law is specified with both this command and others, such as **`hden, constant pressure`**, etc, only the last command will be honored.

It is possible to specify a change in densities so extreme that the code will have convergence problems. Cloudy works by linearizing all equations. It is possible to specify a change in the density that is so extreme that conditions change too much for the solvers to converge. The code uses adaptive logic to adjust the zoning and should prevent this from happening but the heuristics may be fooled by drastic density laws. The code will generate a warning if the density does change by too much – if this happens the cure is to not use such large density contrasts.

8.3.1. dlaw p1, p2, p3 ...

This is the default form of the command. It passes the parameters on the command line to a user-provided function. There are up to ten parameters. A new function ***fabden*** must be written by the user and the version of ***fabden*** already in Cloudy must be deleted. (The code will stop if the initial version of ***fabden*** is not replaced.) Cloudy will call ***fabden*** as needed to determine the density as a function of depth. The arguments of the function are the radius and the depth (these are defined on page 8 above). Both are in centimeters and are double precision variables. The function must return the hydrogen density (cm^{-3}) as a double precision variable. The code provided in the function must use the ten or fewer parameters in the structure ***dlaw*** to compute the density at the current position

The following is an example of a function in which the density is the product of the first number on the command line and the depth.

```
/*fabden called by dlaw command, returns density for any density law */
#include "cddefines.h"
#include "dlaw.h"
#include "fabden.h"

double fabden(double radius, double depth)
{
	return( depth*dlaw.DensityLaw[0] );
}
```

8.3.2. dlaw table [depth, radius]

If the keyword **`table`** appears on the **`dlaw`** command then the code will read in a set of ordered pairs of radii and densities. The original form of this option was added by Kevin Volk. There must be two numbers per line as in the example below.

The first number is the log of the radius or depth [cm] and is followed by the log of the hydrogen density [cm^{-3}]. If the keyword **`depth`** also appears on the command line then the first number is interpreted as the log of the depth from the illuminated face and the table must begin with a depth smaller than 10^{-30} cm, the first point where the depth is evaluated. The first number is interpreted as the log of the radius if **`depth`** does not appear. The ordered pairs end with a line with the keyword **`end`** in columns 1 through 3. Up to 500 pairs may be entered.

Linear interpolation in log-log space is done. The following is an example.

```
dlaw table depth
continue -35 4
continue 12 4
continue 13 5
continue 14 6
continue 15 7
end of dlaw
```

Be sure that the first and last radii or depths extend beyond the computed geometry - this law is only be used for interpolation and the code will stop if extrapolation is necessary. Note that the first depth must be smaller than 10^{-30} cm, and also that there must not be a space in the first column of any lines with numbers – the code will think that an end of file has been reached. Alphabetic characters can be placed anywhere on the line and will be ignored – I placed the word **`continue`** in the first four columns for this reason (it is actually totally ignored).

8.4. fluctuations density period . . . . .

This specifies a density that varies as a sine wave. It was introduced to investigate the effects of inhomogeneities upon the emission-line spectrum (see Mihalszki & Ferland 1983; Kingdon & Ferland 1995). The first number is the log of the period *P* of the sine wave in centimeters. The second two numbers are the logs of the largest and smallest hydrogen densities over the sine wave. Order is important here. The last optional number is a phase shift φ (in radians) which allows the initial zone to occur at any part of the sine wave. If it is omitted the calculation will begin at the maximum density. If the phase is set to π the calculation will start at the minimum density.

The density is scaled according to the relation

$$n(r)=\left(\frac{n_{\max}-n_{\min}}{2}\right)\times\cos\left(\Delta r\frac{2\pi}{P}+\varphi\right)+\left(\frac{n_{\max}+n_{\min}}{2}\right)\quad [\mathrm{cm}^{-3}] \qquad (32)$$

where n_{max} and n_{min} are the maximum and minimum densities and Δr is the depth into the cloud, measured from the illuminated face.

The simulation may result in a large number of zones since the code must spatially resolve the density fluctuations. The zone thickness is not allowed to exceed ~0.05 of the period so that each cycle is divided into at least 20 zones. This may result in very long execution times. The total number of zones (this sets the code's execution time) will be at least 20 times the number of cycles over the nebula.

The keyword **`column`** will replace the depth variable in equation 32 with the total hydrogen column density. The period should then be the column density of one cycle. This will more evenly weight the final column density over low- and high-density gas.

The **fluctuations abundances** command (page 57 above) proves a mechanism for varying the gas-phase abundances of the elements.

8.5. globule [density =2, depth =16, power =2]

This produces a density law that would be appropriate for a power-law density gradient irradiated from the outside (see, for example, Williams 1992). The total hydrogen density $n(r)$ is given by

$$n(r) = n_{\mathrm{o}} \left(\frac{R_{scale\,depth}}{R_{scale\,depth} - \Delta r} \right)^{\alpha} = n_{o} \left(1 - \frac{\Delta r}{R_{scale\,depth}} \right)^{-\alpha} \quad [\mathrm{cm}^{-3}] \qquad (33)$$

where n_{o} is the background density outside the cloud, with default value 1 cm^{-3}, and Δr is the depth into the cloud, measured from the illuminated face. The log of n_{o} is the optional first number on the command line. The variable $R_{scale\ depth}$ is the scale depth for the cloud and has a default of one parsec, $R_{scale\ depth}$ = 3.086×10^{18} cm. Other scale depths are specified by the optional second parameter, which must be entered as a log of the scale depth in cm. The optional third argument is the index α, which has the default[16] α = 1. The arguments can be omitted from right to left.

8.6. hden 5.6, [proportional to R -2, ...]

The first number is the log of the total (ionic, atomic, and molecular) hydrogen density at the illuminated face of the cloud. This is the sum

$$n(\mathrm{H}) = n\left(\mathrm{H}^0\right) + n\left(\mathrm{H}^+\right) + 2n\left(\mathrm{H}_2\right) + \sum_{other} n\left(\mathrm{H}_{other}\right) \ [\mathrm{cm}^{-3}] \ . \qquad (34)$$

If the optional keyword **linear** appears then the number is the density itself and not its log.

For situations where the hydrogen atom is close to LTE and the gas is hot, there is a problem in defining the neutral hydrogen density because of the well-known divergence of the partition function, as discussed, for instance, by Mihalas (1978). The atomic hydrogen density is defined as the total population in all computed levels. In most circumstances, i.e., n(H) ? 10^{13} cm^{-3} and $T \le 10^4$ K, the ambiguity is much less than 1%.

Several options are available to specify optional power-law dependencies on depth variables. These are described in the next sub-sections.

8.6.1. Power-law dependence on radius

The second (optional) number is the exponent α for a power-law radial density dependence, as in the following example:

```
hden 9, power =-2
```

[16] The default index was 2 for versions 89 and before.

i.e.,

$$n(r) = n_o(r_o)\left(\frac{r}{r_o}\right)^{\alpha} \text{ [cm}^{-3}\text{]} \ . \qquad (35)$$

In this example n_o, the density at the illuminated face of the cloud, will be 10^9 cm^{-3}. The optional power law is relative to radius, the distance to the central object, not the depth into the cloud. If α = -2 then the density will be proportional to the inverse square of the radius. Both density and photon flux will fall off as an inverse square and the cloud will tend to have the same ionization parameter (and hence physical conditions) across the ionized zone.

8.6.2. Models extending to infinity

For an inverse-square density law there is a critical value of the number of ionizing photons emitted by the central object, corresponding to an ionization front at infinite radius;

$$Q_{crit}(\mathrm{H}) = \alpha_B(T_e) n_o^2 4\pi\, r_o^3 \text{ [s}^{-1}\text{]} \ . \qquad (36)$$

A hydrogen ionization front will not be present and the model will extend to infinite radius when $Q(\mathrm{H}) \geq Q_{crit}(\mathrm{H})$. In this expression $\alpha_B(T_e)$ is the hydrogen Case B recombination coefficient and n_o and r_o are the inner density and radius respectively. Generally, a hydrogen ionization front will not be present if the density falls off faster than an inverse square law, but rather the level of ionization will tend to *increase* with increasing radius. In either case, if a reasonable outer radius is not set, the calculation will extend to very large radii, an unphysically small density will result, and usually the code will crash due to floating point underflow, followed by division by zero. It is usually necessary to set an outer radius when the density falls off with an index $\alpha \leq -2$, since, for most circumstances, the cloud will remain hot and ionized to infinite radius and zero density.

8.6.3. Power-law dependence on depth

The density will depend on the depth into the cloud rather than the radius if both the optional exponent *and* the keyword **depth** appear:

```
hden 9, power =-2, scale depth = 13
```

The density is given by

$$n(r) = n_o(r_o)\left(1 + \frac{\Delta r}{R_{scale}}\right)^{\alpha} \text{ [cm}^{-3}\text{]} \qquad (37)$$

where R_{scale} is the scale depth and Δr is the depth. The log of R_{scale} [cm] is the third number on the line and must be set.

8.6.4. Power-law dependence on column density

The local hydrogen density will depend on the total hydrogen column density if both the optional exponent *and* the keyword **column** appear;

```
hden 9, power =-2, scale column density = 21
```

Here the density is given by

$$n(r) = n_{\rm o}(r_{\rm o})\left(1 + \frac{N(\mathrm{H})}{N(\mathrm{H})_{scale}}\right)^{\alpha} \ [\mathrm{cm}^{-3}] \qquad (38)$$

where N(H) is the total hydrogen column density [cm^{-2}] from the illuminated face to the point in question, and $N(\mathrm{H})_{scale}$ [cm^{-2}] is the scale column density. The log of $N(\mathrm{H})_{scale}$ is the third number.

9. GEOMETRY

9.1. Overview

This section describes commands that determine the geometry of the emission-line region. Many of the quantities used below are defined in the section on geometry starting on page 8 above.

The geometry is always spherical but can be made effectively plane parallel by making the radius much greater than the thickness of the nebula. It is also possible to compute a model in which the emission-line region is almost a disk. A covering or filling factor can be specified and the cloud can be either static or expanding.

9.2. age 44 years [_off]

For a static geometry the code assumes that the cloud is old enough for atomic processes to have become time-steady. The **age** command allows the code to confirm that the microphysics is indeed time steady. The age of the cloud is the number on the command line. The default units are linear seconds. The keyword **_log** will force the code to interpret the number as a log. The keywords **minutes**, **days**, **weeks**, **fortnights**, **months**, **years, centuries**, and **millennia** change the units.

The code keeps track of many equilibrium timescales during a calculation. After the calculation is complete it will check that none of the equilibrium timescales for significant physical processes were longer than the age of the cloud. The code will complain if the age of the cloud is not set but still compute the model. If a physical process is not significant, for instance, the H_2 formation timescale in a highly-ionized gas, the age is set to a negative number. This retains the value while not including the process as a significant part of the physical simulation.

If the keyword **_off** appears then the age will not be checked.

9.3. aperture [slit, beam]

The **aperture** command simulates observing a part of the computed structure with a spectrometer. It was first incorporated into the code by Peter van Hoof who wrote the original version of this section.

One of the keywords **slit** or **beam** must appear. The keyword **beam** tells the code to simulate observing a resolved nebula with a small beam centered on the central star. If the keyword **slit** appears then the computed structure is observed with a slit that is longer than the nebula.

The **aperture** command only affects how volume emissivities are added together to form the final spectrum. It has no effect on any aspect of the calculation of conditions in the gas.

In the following a quantity α is defined with the following meaning: $\alpha = 0$ in the pencil beam case (we are observing along a single line of sight passing through the center of the nebula), $\alpha = 1$ in the long-slit case (we are observing through a narrow slit placed over the center of the nebula; the slit is longer than the nebula and the flux is integrated over the entire slit), and α = 2 in the general case (we are observing the flux integrated over the entire nebula). The default index is $\alpha = 2$.

In all cases an observed quantity Q_α can be defined for a line λ as

$$Q_\alpha(\lambda) = C_\alpha D_\alpha \int \left(\frac{r}{r_o}\right)^\alpha \varepsilon(\lambda) \ \ dr \quad , \tag{39}$$

where $\varepsilon(\lambda)$ is the line's volume emissivity (erg cm^{-3} s^{-1}) and

$$\begin{aligned} C_0 &= 2 \\ C_1 &= 2\pi r_o \quad , \\ C_2 &= 4\pi r_o^2 \end{aligned} \tag{40}$$

where r_o is the inner radius of the nebula. The covering factor D_α depends on the geometry and is

$$\begin{aligned} D_0 &= 1/2,\ 1 \\ D_1 &= \Theta/2\pi \quad . \\ D_2 &= \Omega/4\pi \end{aligned} \tag{41}$$

For the entire nebula (α = 2) this is the familiar definition. In the long slit case (α = 1) D_1 is the fraction of a large circle in the plane that is being observed that actually passes through nebular material. In the beam case (α = 0) D_0 indicates whether only the front or back side of the line of sight is covered with nebular material (D_0 = 1/2) or if both sides are covered (D_0 = 1). The covering factor for the entire nebula is set with the **`covering factor`** command (see page 77 below) – it is not now possible to set the covering factor in the long slit case.

This command only affects the line luminosities in the luminosity case (see page 10 above). When the intensity case is used and the inner radius is not specified all integrations are for a pencil beam through the slab. In the luminosity case Q_α will have units erg s^{-1} for the entire nebula, erg cm^{-1} s^{-1} for the long slit case, and erg cm^{-2} s^{-1} for the beam. In the intensity case the units are erg cm^{-2} s^{-1}. See page 10 above for a discussion of the luminosity and intensity cases.

In the luminosity case we can also construct relations between observed quantities and the quantities predicted by the code. These neglect interstellar extinction of course. The flux measured at the Earth will be

$$F_\alpha(\lambda) = \frac{A_\alpha}{4\pi D^2} Q_\alpha(\lambda) \ \ \text{[erg cm}^{-1}\text{ s}^{-1}\text{]}, \tag{42}$$

with

$$\begin{aligned} A_0 &= \Omega_b D^2 \\ A_1 &= \Theta_s D \quad . \\ A_2 &= 1 \end{aligned} \tag{43}$$

Here F_α is the observed flux in erg cm^{-2} s^{-1}, D is the distance of the object (cm), as specified with the **distance** command (page 78 below), Θ_s is the slit length in radians, and Ω_b is the surface area of the pencil beam in sr.

In the intensity case (the intensity case implies α = 0) the relation between the observed surface brightness $S(\lambda)$ and $Q_o(\lambda)$ is simply:

$$S(\lambda) = \frac{\Omega\left(1\ \mathrm{arcsec}^2\right)}{4\pi} Q_0(\lambda) \approx 1.87043\times 10^{-12} Q_0(\lambda)\ [\mathrm{erg\ cm^{-2}\ s^{-1}\ arcsec^{-2}}]\ . \qquad (44)$$

For the case where both sides of a spherical shell are observed, $S(\lambda)$ will be twice this.

9.4. covering factor 0.3

This sets a covering factor $\Omega/4\pi$ for the emission-line region (see AGN3 section 5.9). The argument is interpreted as the log of the covering factor if less than or equal to zero, and the covering factor itself if positive. It is impossible to specify a covering factor of zero.

The covering factor affects both the luminosity of the emitted spectrum and the radiative transfer of lines and continua. If a covering factor is set and the luminosity case (see page 10 above) used then the luminosities will be for a shell covering Ω sr of the central object. Line luminosities will scale nearly linearly with the covering factor. The covering factor does not strongly affect the line intensities in the intensity case, where the emission per unit area of cloud is considered. The covering factor does have second-order effects on the spectrum because of changes in the transport of the diffuse fields.

This covering factor is referred to as the geometric covering factor, and is stored as the variable ***covgeo***. A second covering factor, ***covrt***, affects the transfer of lines and continua. This command sets both covering factors.

If no covering factor is entered and **sphere** is not set then the default is for a geometric covering factor of unity (the shell fully covers the continuum source) but a radiative covering factor of zero (i.e., an open geometry).

9.5. cylinder log semi height =9.12

The model will be spherical, but truncated so as to simulate a cylinder (see Ferland et al. 1982). Figure 8 gives an example of the assumed geometry.

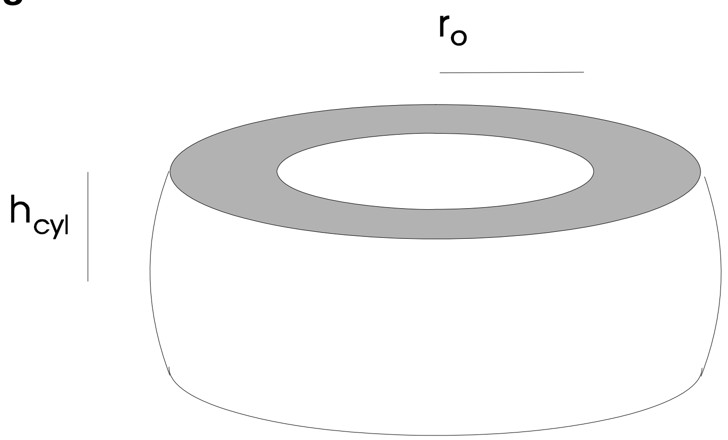


Figure 8 This figure shows the geometry assumed when the cylinder command is used. cylin

The inner and outer radii of the cylinder are set by the **radius** command described on page 79 below. The **cylinder** command sets the full height of the cylinder to twice the number entered on the command. The argument is the log of the semi-height in cm.

The effective volume element used to compute the emissivity of the gas is given by

$$dV = 4\pi\, r_o^2 \left(\frac{r}{r_o}\right)\left(\frac{\min\left(r, h_{cyl}\right)}{r_o}\right) f\left(r\right) dr \quad [\mathrm{cm}^{-3}] \tag{45}$$

where r_o is the inner radius, h_{cyl} is the cylinder half-height, and $f(r)$ is the filling factor. The default value is $h_{cyl} = 10^{35}$ cm.

Changing the emissivity as described by equation 45 is the only effect of this command. It does not alter the radiative transfer methods and is only formally correct when the continua and lines are optically thin.

9.6. distance 3.2 linear parsecs

This sets the distance to the object from the Earth. The number is the log of the distance in centimeters. The **linear** keyword forces the number to be interpreted as the linear distance and the **parsecs** keyword changes the units to parsecs.

If the distance is set then it is possible to predict the emission-line fluxes observed at Earth if the luminosity case (see page 10 above) is computed. The code must have enough information to predict emission-line luminosities (see the discussion on page 10 above) to do this. If the code can predict luminosities and the distance is set then the observed emission-line fluxes at the Earth will be printed if the **print line flux** command (135 below) is also entered.

This command can be combined with the **aperture** command (page 75 above) to simulate observing parts of a nebula from the Earth.

9.7. filling factor = 0.05 [index =-1]

The first number is the filling factor $f(r)$ for a clumpy model (AGN3 Section 5.9). It can be either the filling factor itself (which is greater than zero and less than or equal to one) or the log of the filling factor (if it is less than or equal to zero). The second optional number is the index α for a power-law variation of the filling factor $f(r)$, i.e.,

$$f\left(r\right) = f\left(r_o\right)\left(\frac{r}{r_o}\right)^{\alpha} \tag{46}$$

where r_o is the inner radius of the cloud.

The filling factor is used in two ways. The first is to modify the volume emissivity of the gas,

$$dE = \varepsilon\, f\left(r\right)\, dV \frac{\Omega}{4\pi} \quad [\mathrm{erg\ s}^{-1}] \tag{47}$$

where $\Omega/4\pi$ is the covering factor. The second is to modify the optical depth scale

$$d\tau = \alpha_{l,u}\left(n_l - n_u \frac{g_l}{g_u}\right) f(r)\, dr \qquad (48)$$

(see Osterbrock and Flather 1959).

A filling factor greater than unity is not allowed. Cloudy will set a filling factor of unity if a value greater than one is entered. The code will complain (but compute the model) if a filling factor is set in a constant pressure model since this makes no physical sense.

9.8. illumination angle 45 deg [radians]

The plane-parallel slab is illuminated by a beam θ away from the normal. The default is $\theta = 0$ (normal illumination). The angle is in degrees unless the keyword **radian** appears.

The only effect of this command is to cause the beam of incident radiation to be attenuated by $\tau_n / \cos(\theta)$ where τ_n is the normal optical depth of the zone. The line and diffuse continua optical depth scale, which is defined normal to the plane, are not directly affected by this command.

N.B. If this is used with the **grid** or **vary** options the angle must be given in radians. See the discussion starting on page 183 below.

9.9. radius r(inner) [r(outer), thickness; parsec; linear]

The first number is the log of the inner radius. The second optional number sets a stopping radius and is either the log of the outer radius (if it is larger than the first number) or the log of the thickness of the cloud (if it is less than or equal to the first number).

The numbers are normally interpreted as the log of the radii in cm. If the optional keyword **linear** appears then the numbers are interpreted as linear numbers. The default units are centimeters. The arguments will be interpreted as the log of the radii in parsecs if the keyword **parsec** appears. Arguments will be interpreted as linear parsecs if both keywords appear. The following gives examples of its use.

```
radius 19.5       // log of inner radius in cm
radius 19.5 18.5  // as above, but a thickness of 3x10^18 cm
radius 19.5 20    // inner radius as above, outer radius 10^20 cm
radius 100 linear // inner radius of 100 cm
radius 0 parsecs  // log of radius in parses, so inner radius 1 pc
radius 1 to 3 linear parsecs // inner radius 1 pc, outer 3 pc
```

The default outer radius is effectively infinite (actually 10^{31} cm). If the intensity case is used then a starting radius of 10^{30} cm will be set by default. Under most circumstances this will result in a plane-parallel geometry.

Page 184 below describes a problem that can occur if the second parameter is used with the **vary** option. Please read it if you will vary the radius with the outer radius set.

The **stop thickness** command (page 126 below) provides another way to set a stopping thickness without specifying a starting radius.

9.10. sphere [options][17, 18]

Cloudy normally assumes an open geometry (defined on page 9 above), i.e., that the gas covering factor is small. The **sphere** command should be included to change this assumption for a closed geometry (defined on page 9 above), one where the covering factor of the gas is large and the model spherical. This command tells Cloudy to take into account ionization by the diffuse continua and lines produced in the far side of the nebula (i.e., from beyond the central object), and not to attenuate the ionizing continuum by pure scattering opacities, such as electron scattering, back scattering by grains, or Rayleigh scattering.

This option should be set when the geometry is spherical and gas nearly fully covers the continuum source. It should not be set when the covering factor is small so that emission from a cloud is unlikely to encounter another cloud. This latter case is the default. In the language of Van Blerkom and Hummer (1967), **sphere** causes Cloudy to assume the symmetric case (their equation 2.14), rather than the default zero case (their equation 2.13) for diffuse continua. Here these are referred to as closed and open geometries, respectively.

Situations can occur where it is not obvious whether or not **sphere** should be used. In this case it would be best to compute models with and without **sphere** and compare results. In most cases this will only make a 10 – 15% difference in predicted quantities.

9.10.1. sphere expanding or static

Two optional keywords, **expanding** and **static,** determine how line transfer is handled. If **expanding** (the default when **sphere** is entered) is set then Cloudy assumes that line photons escaping from the illuminated face of the cloud are Doppler shifted away from lines of absorbing material on the far side of the shell. This will be the case if the expansion velocity exceeds the Doppler width by large amounts. If **static** is set then line photons *do* interact on both sides so that even line photons produced at the illuminated face of the cloud will be strongly trapped by material on the far side. Lα radiation pressure in the H^+ region will probably be significant if **sphere static** is set and grains are not present.

It is necessary to iterate at least one time when the **static** option is used since the total line optical depths are not known on the first iteration. All optical depths are determined self-consistently on second and further iterations.

The specific effects of **sphere** are the following: The total continuous optical depths are assumed to be twice the computed optical depths, and the initial optical depth is half the total. All diffuse reemission (bremsstrahlung, free-bound, etc.) is

[17] The **slit** and **beam** options were recognized by the **sphere** command before version 96. These options were moved to the **aperture** command which was introduced in version 96.

[18] Before version 96 the **sphere** command included an option to change the covering factor. The covering factor was removed from the **sphere** command. Only the **covering factor** command changes the covering factor.

counted in the outward beam rather than only half. Scattering opacities are not considered in the attenuation of the incident radiation field. When **`static`** is set, the optical depth in Lα in the inner direction is set to 10^5 on the first iteration. Otherwise it is 10^{-20}. The total optical depths of lines are twice their computed depth for the static case. Finally, ionization by lines and continua produced in the other side of the nebula is included. At the end of the iteration all inward optical depths are set to half of the total value computed from the previous iteration. The diffuse continua are transferred using methods described in later sections.

9.11. stop depth …

9.12. stop thickness …

These commands provide methods to set the thickness of a cloud without specifying its radius. They are described on page 126 below.

10. OPTICAL DEPTHS AND RADIATIVE TRANSFER

10.1. Overview

Line transfer is relatively unimportant in nebulae such as H II regions and planetary nebulae. Radiative transfer can be important in other environments, such as nova shells and the broad-line region of active nuclei, where excited states of hydrogen have significant populations and subordinate lines become optically thick. In other cases grains are present and all lines can be absorbed by background opacity. All radiative transfer effects are included in the treatment, including line thermalization, destruction by background opacities, pumping by the incident continuum, and escape from the cloud. Further details are given in Part 2 of this document.

It is necessary to iterate upon the solution if emission lines are optically thick since total optical depths are not known on the first iteration. The default is for a single pass through the cloud. This is often adequate for low-density nebulae such as planetary nebulae or H II regions. A second iteration is sometimes enough to establish a fairly accurate line optical depth scale for most resonance transitions. Further iterations are usually needed when subordinate lines are also optically thick. The program has an **`iterate to convergence`** command (page 99 below) to iterate until the optical depth scale is well defined.

Line-radiation pressure cannot be computed accurately until the total line optical depths are known, so this quantity is only meaningful after the first iteration. Cloudy will stop if the internal radiation pressure exceeds half of the surface gas pressure in a constant-pressure model since such a geometry is unstable unless it is self-gravitating. The radiation pressure is not allowed to exceed half the gas pressure on the initial iterations of a multi-iteration constant-pressure model. This is to prevent the calculation from stopping when the optical depth scale is not yet well converged.

The following subsections outline various commands that affect the radiative transfer and discuss several of the model atoms that are available.

10.2. atom overview

The **`atoms`** commands change details of the physical treatment of several model atoms that are incorporated in the code.

10.3. atom CO [options][19]

Rotational transitions within the ground electronic – vibration state of CO are treated as a rigid rotor. This is a single implementation that currently includes ^{12}CO and ^{13}CO. (The ^{13}CO chemistry is not now done – the ^{12}C/^{13}C ratio is set with the **`set 12C13C`** command described on page 206 below).

[19] This command was the same as atom rotor. The atom rotor command was removed in C07 although it is still accepted for now.

10.3.1. atom CO levels 25

This sets the number of rotation lines (not levels) in the rigid rotor molecules. There will actually be one more level than line, to include the upper level of the highest rotation transition. There is no limit to the number of lines that can be included. The default is 20.

A problem can occur if too few levels are used. The lower rotation transitions of CO are often optically thick because of its great abundance. The cooling will shift to higher levels as a result. If the molecule is too small then the level populations will pile up into the highest levels. The cooling will be underestimated and the transition to the highest level may develop an artificial maser. The code will check for this and generate a caution if it occurs. If this happens the model should be recomputed with more levels.

The number of levels can only be set once at the very start of a calculation when space is allocated for the rigid-rotor line arrays. If the code is used to run a grid of models only the first occurrence of **`atom CO levels`** will be honored and all following occurrences ignored.

10.4. atom FeII [options]

This command adjusts details of the model Fe^+ ion. The default is to compute the lowest 16 levels, which produce IR emission, as in the real ion, but to do higher levels, which produce optical and UV emission, using the simplified and very fast scheme outlined by Wills, Netzer, and Wills (1985). AGN3 describes Fe II emission in section 14.5.

When any of the **`atom FeII`** commands are entered the Wills et al. scheme is turned off. A complete model, using 371 levels and described by Verner et al. (1999), is used instead. This is far more accurate but also *much* slower. Baldwin et al. (2004) show some examples of Fe II spectra of AGN.

N.B. the keyword is **`FeII`**, not **`Fe2`**, to avoid scanning the number 2 off the command line. Both **`FeII`** and **`Fe_II`** (with a space) are accepted.

10.4.1. atom FeII levels

This changes the number of levels used by the model atom. The upper limit is 371 levels and is the default when the large FeII model is used. When the large atom is not used the default is to compute the lowest 16 levels and treat the remainder of the levels with the Wills et al. (1985) simple model. Decreasing the number of levels will speed up the execution time [roughly proportional to $n^2 \log(n)$] at the expense of a degraded simulation of the physics.

10.4.2. atom FeII trace

This turns on debugging printout for each call to the model atom.

10.4.3. atom FeII redistribution [options]

The keyword **`redistribution`** will change the form of the redistribution function for various lines within the model atom.

A keyword to specify which set of lines to change is required. This is either **resonance** (any line decaying to the ground term) or **subordinate** (transitions between excited states). The type of redistribution function to use is also specified. The options are **_PRD** (partial redistribution), **_CRD** (complete redistribution with Doppler core only), and **CRDW** (complete redistribution with damping wings). (The underscore indicates a space.)

The keywords **redistribution show** tells the code to print the current default redistribution functions.

10.4.4. atom FeII simulate

This will cause results from the atom to be simulated. The large model atom is not actually called. This is very fast and is a debugging aid.

10.4.5. atom FeII slow

The keyword **slow** will cause the atom to always be reevaluated. Normally the code only reevaluates the atom when the local conditions have changed significantly.

10.4.6. atom FeII output options

Fe II emission is an exercise in uncontrolled complexity. Hundreds of thousands of lines contribute to what often appears as a pseudo-continuum. It is not practical to simply list the lines except in a few especially simple situations such as H II regions.

Three options are available for understanding output from the Fe II atom. Most often Fe II emission is seen as a blended continuum rather than individual lines. The general idea is to try to reduce the flood of information to a manageable level by distilling the emission into what an observer would actually see.

Fe II bands in the main output. A series of Fe II “bands” are automatically entered into the main emission-line output when the large Fe II atom is used. Each band represents the total Fe II emission integrated over all lines that lie within a range of wavelengths. This emission appears in the output with the label “Fe2b” and a wavelength close to the center of the band. The bands are chosen to represent features that an observer might be able to measure.

The list of bands is contained in the file *bands_Fe2.dat* which is included in the data directory. This file is intended to be easily changed by the user. It explains the format of the information that is needed. There is no limit to the number of Fe II bands that can be specified.

punch FeII lines This option punches the intensities of all emission lines predicted by the model atom. The resulting file is very large and mainly useful for debugging the model atom or understanding where within the atom a particular feature originates. **Punch** commands are described in more detail beginning on page 138 below.

punch FeII continuum This option punches the total Fe II emission as a continuous spectrum. Here a range of wavelengths is broken into a number of intervals and the total Fe II emission within each interval is added together. The result represents what would be observed by a spectrometer with a particular resolution and was used to create the plots in Baldwin et al. (2004). This command is described further on page 151 below. **`Punch`** commands are described in more detail beginning on page 138 below.

atom FeII continuum from 1000Å high to 7000Å in 1000 cells This adjusts the lower and upper bounds and the resolution of the Fe II continuum punched with the **`punch FeII continuum`** command. The numbers are the lower and upper limits to the wavelength range in Angstroms and the number of wavelength cell that occur over this range.

10.5. atom H2 options

The large model of the H_2 molecule, described in Shaw et al. (2005), will be included if any of the family of **`atom H2`** commands appears. The much faster three-level model outlined by Tielens & Hollenbach (1985a), Burton, Hollenbach & Tielens (1990) and Draine & Bertoldi (1996), and expanded by Elwert et al. (2006), is used by default. The large molecule is represented by several thousand levels producing roughly half a million lines. AGN3 describes some properties of H_2 in section 8.3 and appendix A6.

NB The number "2" appears in the keyword for this command. Any numerical parameters that appear on the **`atom H2`** commands must appear after this two – the code will check that the first number parsed off the command line is the number 2.

10.5.1. The "set H2" command

Some details of the physical treatment of the H_2 molecule can be changed with the **`set H2`** command, described on page 211 below.

10.5.2. H_2 output options

Strong H_2 lines will appear in the main emission line output. The **`punch H2`** command (page 155 below) has many other output options. The section in Part 3 of this document describing calling the code as a subroutine describes several routines that will return predictions of the large molecule. The **`set line precision`** command (page 213 below) will add another significant figure to the wavelengths printed in the main printout. This may help isolate a particular line.

10.5.3. atom H2

With no options, the only effect is to include the large model of the H_2 molecule.

10.5.4. atom H2 chemistry [simple; full]

This changes how the interactions between the H_2 molecule and the rest of the chemical network are treated. By default, or if the keyword **`full`** appears, then the fully self-consistent formation and destruction rates are used when the large H_2 molecule is enabled. If the keyword **`simple`** occurs then expressions from Tielens & Hollenbach (1985a) are used instead.

10.5.5. atom H2 collisions [options]

This changes various collisional processes within the H_2 molecule. The commands have keywords **`_ON`** and **`_OFF`** to turn the process on or off. The default, when neither is present, is to disable the process.

`atom H2 ortho para collisions on/off` turns off ortho-para changing collisions with gas particles .

`atom H2 collisional dissociation on/off` turns on or off collisional dissociation. The default is to include it using the estimates given in Shaw et al. (2005). These rates are all only guesses and represent an uncertainty.

`atom H2 grain collisions on/off` turns off downward transitions induced by collisions with grains.

By default the code will uses guesses of collisional rate coefficients using the g-bar method. Collisional deexcitation for the g-bar transitions are turned off with the **`atom H2 gbar`** command.

10.5.6. atom H2 gbar [off; on]

The g-bar approximation is a rough relationship between the energy of a line and its collision rate coefficient. This can be used to guess a collisional deexcitation rate coefficient when no calculated data exist. This command turns this guess off or on. It is on by default.

10.5.7. atom H2 levels

This changes the number of electronic levels within the H_2 molecule. The default is seven and includes the ground and first six bound singlet electronic states. This is also the largest number of levels. At minimum is three levels, which is sufficient to include the Lyman and Werner bands in the UV. This are a necessary minimum number of levels to include the correct photodissociation processes. If no number appears but the keyword **`large`** does then the code will use the upper limit.

10.5.8. atom H2 limit -4

Calculating the level populations and line spectrum of the large H_2 molecule is computationally expensive. The code tries to save time by not computing the populations when the abundance of H_2 is negligible. This command changes the limit for the smallest H_2/H_{tot} ratio. The full model will be computed when the ratio is greater than this limit. The number is interpreted as the linear ratio if it is greater than zero and the log of the ratio if it is less than or equal to zero. The keyword **`_off`** turns off the limit so that the large model of the molecule is always evaluated. The default limit is 10^{-8}, small enough for the large molecule to be computed across the entire Tielens & Hollenbach (1985a) standard PDR model that is part of the code's test suite.

When the H_2 abundance is below this limit the photodissociation, heating, and cooling rates, are evaluated using expressions in Tielens & Hollenbach (1985a). H_2 level populations are set to their LTE value so that self-shielding in the electronic bands is still computed.

10.5.9. atom H2 matrix 43

Populations of the lower ro-vibration states of the ground electronic level are determined by two schemes. The first, and most straightforward, is the solution of a complete set of balance equations by solving the system of balance equations in a matrix. The time needed to solve the linear algebra increases as a power of the number of levels, so we need to keep the number of levels as small as possible. High levels are treated by back substitution, starting from the highest level with X and proceeding downwards. This command sets the total number of levels that are computed within the matrix. Levels higher than this will be treated with back substitution.

If the keyword **`_off`** (note the leading space) or **`none`** appears, or if the number of levels is less than 1, the matrix will not be used. It the keyword **`_all`** appears then all levels within X will be done this way.

10.5.10. atom H2 noise [mean, standard deviation, seed]

This multiplies the rates for collisional processes within the H_2 molecule by a Gaussian random number so that $r' = r\,10^{\mathrm{rand}}$. Here *r* is the correct rate coefficient and ***rand*** is an Gaussian distributed random number. The first two optional numbers on the command line set the mean and standard deviation for the Gaussian random numbers. The first optional number is the mean, with a default of 0. The second optional number is the standard deviation with a default of 0.5. The last optional number is the seed for the random number generator, which must be an integer greater than 0. If the seed is not specified then the system time is used to generate a random seed.

10.5.11. atom H2 thermal [simple; full]

This changes how the heating and cooling by the H_2 molecule are treated. By default, or if the keyword **`full`** appears, then the fully self-consistent heating and cooling rates are used when the large H_2 molecule is enabled. If the keyword **`simple`** occurs then expressions from Tielens & Hollenbach (1985a) are used instead.

10.5.12. atom H2 trace [options]

This turns on trace information concerning the H_2 molecule. The optional keywords **`full`**, **`iterations`**, and **`final`** will give full information, an overview of iterations during the convergence, and only final results respectively. If the keyword **`matrix`** occurs the code will print the contents of the matrices that are used for solution of lower levels within the ground electronic state.

10.5.13. atom H2 output options

Roughly half a million lines are predicted when the large H_2 molecule is included. The main emission-line printout includes all significant lines produced in the ground electronic state but does not include electronic transitions. The **`print line H2 electronic`** command (page 136 below) will include these lines. The family of **`punch H2`** commands (page 155 below) provides ways to save information such as column densities, the emission-line spectrum, and details of the effects of H_2 on the conditions in the cloud.

10.6. atom H-like [options]

10.7. atom He-like [option

These are used to change some details in the treatment of atoms of the hydrogenic and He-like isoelectronic sequences. Atoms of the H-like sequence have one bound electron and include H^0, He^+, Li^{+2}, through Zn^{+29}.[20] Atoms of the He-like sequence have two bound electrons and include He^0, Li^+, through Zn^{+28}.

This implementation of the H-like sequence was initially part of Jason Ferguson's PhD thesis and is described in Ferguson & Ferland (1997), Ferguson et al. (2001), and Bottorff et al. (2002). The physics was expanded to resolve *nl* terms by Ryan Porter. Any number of levels up to *n* of 400 can be computed. The He-like sequence was developed by Ryan Porter as part of his thesis and it is described in Bauman et al. (2005), Porter et al. (2005), and Porter & Ferland (2007). Ryan Porter unified the two sequences and expanded the H-like sequence to include all of the physics included in the He-like sequence.

The two sequences are now unified so the same atom xx-like commands work for both. One off the iso-sequences must appear on the command line. The keywords are H-like and He-like. Only one iso-sequence can be modified with a single command. If the name of an element does not also appear then the entire iso-sequence will be changed. If the name does appear then only that atom is modified. The following are some examples

```
c only change hydrogen itself
atom H-like hydrogen levels 8
c change the entire He-like sequence
atom He-like levels 9
```

The model atoms include a certain number of resolved and collapsed levels. The lower $n_{resolved}$ levels are *nl* resolved. Another $n_{collapsed}$ levels, which replace the nl terms with an n configuration, are above the resolved levels. The physics of the resolved levels is exact while that of the collapsed levels is more approximate since the entire n configuration is treated as a single level. By default only lines produced by resolved levels are included in the printout.

10.7.1. atom H-like collisions . . . .

Collisional processes, both between levels ionization, are turned off with this command. They are all on by default. This command is mainly used for debugging. Separate collisional processes can be turned off with the following options. Only one option is recognized per command line so multiple commands are needed to turn off several processes. If no sub-options are recognized then all collisional processes are disabled. This command turns off collisions for all elements along the H-like isoelectronic sequence.

[20] This was the **hydrogenic** command in versions 90 and before of the code.

atom H-like collisions l-mixing off[21] This turns off *l*-mixing 2*s*-2*p* collisions.

atom H-like collisional ionization off This command turns off collisional ionization by thermal electrons of all levels, except for the very highest level. Collisional ionization from the highest level is not turned off to allow the atom to have some coupling to the continuum. Ionization by cosmic rays is not affected by this command.

atom H-like collisional excitation off This command turns off collisional excitation of all levels, except for 2s-2p.

atom H-like collisions off All three collisional processes will be turned off if none of the three keywords are recognized.

Warning! The code will require a very number of zones if collisions are turned off in an optically thick cloud with a large ($n \cong 15$) hydrogen atom. Collisions will normally hold populations of very highly excited levels to values very near LTE. The FIR and radio lines will have very small line optical depths due to the correction for stimulated emission. When collisions are absent, the normal tendency of departure coefficients to increase with principal quantum number means that FIR and radio lines will strongly mase. The code dynamically adjusts the zoning to prevent these maser optical depths from diverging to minus infinity. A very large number of zones will be required to spatially resolve the masing region. This is a totally artificial, not physical, effect. The solution is to not turn off collisions with a large atom when performing a simulation with more than a trivial thickness.

10.7.2. atom H-like damping off

Rayleigh scattering, continuum scattering due to the extreme damping wings of Lyman lines, can be turned off with the **`damping off`** option. Rayleigh scattering is a significant opacity source in clouds that have large column densities of neutral material ($N(H^0) > 10^{23}$ cm^{-2}).

10.7.3. atom H-like levels 15 [element iron]

This sets the number of levels. The atom can extend up to any principle quantum number between the limits $4 < n \le 400$. The size is limited mainly by the available memory and computer time. Note that there will actually be n+1 levels in the calculation since the 2*s* and 2*p* states are treated separately. The default highest quantum level is n = 15. Increasing the number of levels allows a better representation of the collision physics that occurs within higher levels of the atom at the expense of longer execution times and greater memory requirements.

If no number appears on the **`atom H-like levels`** command, but the keyword **`large`** or **`small`** does, then either 50 or 10 levels will be used. If the keyword **`very small`** also appears then the smallest possible atom, up to n = 4 to include Hβ, is

[21] This was the 2s2p option in versions 94 and before. The 2s2p option still exists for backward compatibility.

computed. These keywords provide a version-independent method of insuring that the code uses the largest or smallest possible number of levels.

By default this command changes all elements along the hydrogenic isoelectronic sequence. If the keyword **element** appears together with the name of an element, only the model atom for that particular element will be changed. For example, the following would set the full isoelectronic sequence to a small number of levels, then reset hydrogen, helium, and iron to a large number.

```
atom H-like levels small
atom H-like levels large element hydrogen
atom H-like levels large element helium
atom H-like levels large element iron
```

The number of levels can only be set once at the very start of a calculation when space is allocated for the hydrogenic arrays. If the code is used to run a grid of models then only the first occurrence of **atom H-like levels** is honored and all following occurrences are ignored.

Warning! Note that the command

```
atom H-like levels large
```

will set all 30 hydrogenic atoms to a large number of levels. This would require roughly half a gigabyte of memory for the H-like sequence along, and would be very slow on today's computers. It is best to set only the most important elements to large levels.

10.7.4. atom H-like Lyman lines

This set of commands changes the treatment of the H I Lyman lines.

atom H-like Lyman pumping off turns off continuum radiative pumping of the Lyman lines of H I. This is meant to take into account the possible presence of Lyman lines in absorption in the incident continuum. This command only changes H I and not the entire H-like sequence.

atom H-like Lyman pumping scale 3 The continuum radiative pumping rate of the Lyman lines of H I will be multiplied by the scale factor that appears on the line. This is meant to take into account the possible presence of Lyman lines in emission or absorption in the incident continuum. The pumping rate is normally set by the intensity of the coarse continuum at the line wavelength. This number that appears on the command line is a scale factor that multiplies this continuum. A value of 0 would correspond to totally black Lyman lines. A scale factor of 2 would simulate the presence of stellar Lyman emission lines with peak intensities twice those of the neighboring continuum. This command only changes H I and not the entire H-like sequence.

atom H-like extra Lyman 1000 Atoms and ions of the H-like and He-like isoelectronic sequences use complete multi-level model atoms. The number of levels included is limited mainly by processor speed and available memory. Higher Lyman lines (used here to mean permitted lines that connect directly to ground) have little impact on emission since they scatter and are degraded into Balmer lines and Lα. However, an absorption spectrum will show them as a series of lines converging onto the photoionization continuum from the ground state. The code includes a large number of "extra" Lyman lines, included as absorbers with optical depths output with the **punch line optical depth** command (page 164 below), but not treated as part of the multi-level atoms. The default number of higher Lyman lines is 100, and this can be changed to any number with this command.

10.7.5. atom H-like matrix [lowt, populations]

This determines which form of the level population solver to use. The options are **lowt** for the simple solver, using back substitution, that works for extremely low levels of ionization, and **populations** for the exact matrix solution for the populations themselves. The code normally decides this based on experience, but this command provides an option to override the default choices for testing.

10.7.6. atom H-like redistribution [options]

The keyword **redistribution** will change the form of the redistribution function for various lines within the model atom. This command is only used if you are not happy with the default redistribution functions.

A keyword to specify which set of lines to change is required. This is one of **alpha** (the $2p$ – $1s$ transition), **resonance** (any higher Lyman line decaying to the ground term), or **subordinate** (all Balmer, Paschen, etc lines). The type of redistribution function to use must also be specified. The options are **_PRD** (partial redistribution), **_CRD** (complete redistribution with Doppler core only), and **CRDW** (complete redistribution with damping wings). (The underscore indicates a space.)

The keyword **show** tells the code to print the current default redistribution functions.

There is at present a fundamental uncertainty in the computation of the line radiation pressure for transitions such as Lα. For a simple two-level atom with incomplete redistribution, it has long been known that the line-width is proportional to $(a\tau)^{1/3}$ (Adams 1972, Harrington 1973; a is the damping constant). It is also easily shown that for complete redistribution and a frequency independent source function that the line width would be determined by inverting the Voigt function, and hence proportional to $(a\tau)^{1/2}$. Line interlocking, whereby scattered Balmer line radiation broadens the upper level of Lα (Hubbard and Puetter 1985), can alter the line width, as can collisional effects when the density is high enough for distant collisions to broaden the line. These effects cause major differences in radiation pressure and emergent flux (factors of several) for Lα, which can easily have an optical depth of 10^7 - 10^9, when Balmer lines are also optically thick. This command determines which approximation is used. The default condition is incomplete redistribution, which minimizes the line width and radiation pressure. This issue is discussed further in Elitzur and Ferland (1986).

10.7.7. atom H-like TopOff 6 [_add scale]

This sets the lowest level for "topping off" the total radiative recombination coefficient. This is necessary to obtain the correct total radiative recombination rate coefficient with a finite number of levels. Because only a finite number of levels can be computed the sum of the total recombination coefficient will be less than the sum to infinity. This difference must be added somewhere to conserve the total recombination rate. One can choose to either add on the difference (if the keyword **_add** appears) or scale them (if **scale** appears). The default is **atom H-like topoff 11 scale**, which rescales the recombination coefficient from levels $n = 11$ through the highest level, so that the sum is correct.

This "top off" disturbs the model hydrogen atom since those levels with the extra recombination coefficient have unphysically large recombination rates. This often causes artificially strong masers. The command changes the lowest level with the extra recombination and was introduced for testing. The code will not predict any lines that include these disturbed levels.

This command has been removed

10.8. atom He-like [options]

The following commands change treatments of some of the physical details of how the models of atoms along the He-like isoelectronic sequence (the species He^0, .. C^{+4}, N^{+5}, etc.). Details are given in Bauman et al. (2005), Porter et al. (2005), and Porter et al. (2007).

10.8.1. atom He-like collapsed levels x

This sets the number of collapsed levels, the high-*n* levels that are assumed to be well *l* mixed and hence can be treated without full consideration of *L* and *S* states. This is faster than solving for the resolved states, but the *l*-mixed approximation is only correct at higher densities. One is the minimum number of collapsed levels, as well as the default.

10.8.2. atom He-like collisions ....

Collisional processes between levels and collisional ionization are turned off with this command. Separate collisional processes can be turned off with the following options. Only one option is recognized per command line so multiple commands are needed to turn off several processes. If no sub-options are recognized then all collisional processes are disabled. This command turns off collisions for all elements along the He-like isoelectronic sequence.

atom He-like collisions l-mixing off This command turns off all collisions within the same *n* level for all elements in the helium-like isoelectronic sequence. Both *L*- and *S*-changing collisions are turned off.

atom He-like collisions l-mixing Pengelly [Vrinceanu] This changes to the Pengelly & Seaton (1964) formalism rather than currently the default, based on Vrinceanu & Flannery (2001) for $L > 2$.

atom He-like collisions l-mixing thermal [averaging, no averaging] The **no thermal averaging o**ption calculates the Vrinceanu & Flannery (2001) collision strengths at an impact energy equal to kT, rather than averaging over a Maxwellian distribution. This is the default when a small atom is used. Thermally averaged collision strengths are used when the atom is large.

atom He-like collisions excitation This command turns off collisional excitation, for all $n_u \neq n_l$ transitions, for all elements in the helium-like isoelectronic sequence.

10.8.3. atom He-like dielectronic recombination [off]

This option turns dielectronic recombination off for the entire isoelectronic sequence. Dielectronic recombination is included by default. This command has no effect without the **`_off`** option.

10.8.4. atom He-like error generation X

Monte Carlo error analyses can be performed with this command. Randomly generated Gaussian errors are applied to atomic data. The parameter X is an integer used to set the seed of the random number generator. See Porter et al. (in preparation) for details.

10.8.5. atom He-like FSM

For $L > 2$, levels with the same n and L but different S are strongly mixed due to the spin-other-orbit interaction. This option modifies transition probabilities to account for this fine-structure mixing. The effect on multiplet emissions is negligible. See Bauman et al (2005) for a discussion and calculation of this effect in a zero-density J-resolved helium atom.

10.8.6. atom He-like gbar options

The code employs various forms of the $\bar{g}$ approximation to fill in collision strengths for those transitions with no quantal calculations. This command changes which approximation is used. The options are **`Vriens`** for the Vriens and Smeets (1980) and **`_off`** to set this to zero.

10.8.7. atom He-like levels 4 [element iron]

This sets the number of n levels. The argument is the principal quantum number n for the highest level. It must be three or greater.

If no number appears on the command, but the keyword **`large`** or **`small`** does, then the number of levels will be large enough to extend to either $n = 40$ or 3. These keywords provide a version-independent method of insuring that the code uses a large or small number of levels. Actually, the atoms are coded so that there is no limit to the number of levels that can be included, other than the memory and computer time requirements.

Another keyword, **`huge`**, is used solely for collisionless Case B calculations, such as those in Bauman et al (2005). It causes Cloudy to bypass some system memory allocation for a faster, less memory-intensive, calculation of radiative-cascade spectra. The code cannot be used for other purposes since it disables everything not directly related to the radiative cascade of helium. Disabling this physics is the only direct effect of this command. It is still necessary to set the desired number of levels.

The model atom resolves n-levels into nLS levels, and the $2\,^3P$ term is split into three $nLSJ$ levels. For a given maximum principal quantum number $n_{\max}$, there will be a total of $n_{\max}^2 + n_{\max} + 1$ nLS levels. The default $n_{\max}$ for He^0 is 6, resulting in 43 *nLS* levels, $n_{\max}$ = 5 for 31 *nLS* levels for C, N, O, Fe, and Zn, and $n_{\max}$ = 3 for 13 *nLS* levels for all remaining elements. For reference, to include all *nLS* levels within the *n* = 2, 3, 4, 5, and 6 levels, the atom will need 7, 13, 21, 31, and 43 levels, respectively. Increasing $n_{\max}$ allows a better representation of the atom's emission, especially the collision physics that occurs within higher levels of the atom, but at the expense of longer execution times and greater memory requirements.

By default this command changes the number of levels for all elements along the He-like isoelectronic sequence. If the keyword **`element`** appears together with the name of an element, only the model atom for that particular element will be changed. For example, the following would set the full isoelectronic sequence to a small number of levels, then reset helium and iron to a large number.

```
atom He-like levels small
atom He-like levels large element helium
atom He-like levels large element iron
```

The number of levels can only be set once at the very start of a grid of calculations. This is because space is allocated for the needed arrays only one time per core load. If the code is used to run a series of models then only the **`atom He-like levels`** that occur in the first simulation will be honored and all following occurrences will be ignored.

The model atom does not give a good representation of lines that come from the highest *n* level, which is always a "collapsed" level. Only lines coming from the first *n* - 1 levels will be printed at the end of the calculation.

Warning! Note that the command

```
atom He-like levels large
```

will set all 29 He-like atoms to a large number of levels. This would require roughly half a gigabyte of memory and would be very slow on today's computers. It is best to set only the most important elements to large levels. Depending on the application, this may be only He itself (when $\approx 10^4$ K gas is considered) or the more abundant second and third row elements (for hot gas and X-ray applications).

There are also collapsed levels – levels that do not resolve *S* or *L* but assume that the states within *n* are well-mixed. These collapsed levels bring together all of the individual *nLS* terms as one pseudo-level. The recombination coefficient into this pseudo-level is the sum of recombination coefficients into the individual terms plus the recombination topoff. Transition probabilities from this pseudo-level are calculated as follows

$$A(n_u \to n_l L_l S) = \frac{\sum\limits_{L_u = L_l \pm 1} g_{L_u S} A(n_u L_u S \to n_l L_l S)}{\sum\limits_{L_u = L_l \pm 1} g_{L_u S}} . \qquad (49)$$

This causes the collapsed level to behave exactly as if it were a set of resolved terms populated according to statistical weight.

10.8.8. atom He-like Lyman 1000

Atoms and ions of the H-like and He-like isoelectronic sequences use complete multi-level model atoms. The number of levels included is limited mainly by processor speed and available memory. Higher Lyman lines (used here to mean permitted lines that connect directly to ground) have little impact on the emission, since they scatter and are degraded in Balmer lines and Lα. However, an absorption spectrum will show them as a series of lines converging onto the continuum from the ground state. The code includes a large number of "extra" Lyman lines, included as absorbers with optical depths output with the **punch line optical depth** command (page 164 below), but not treated as part of the multi-level atoms. The default number of higher Lyman lines is 100, and this can be changed to any number with this command.

10.8.9. atom He-like matrix [lowt, populations]

This determines which form of the level population solver to use. The options are **lowt** for the simple back-substitution solver that works for extremely low levels of ionization, and **populations** for the matrix solutions for the populations. The code normally decides this based on experience, but this command provides an option to override the default choices for testing.

10.8.10. atom He-like no recombination interpolation

The code normally derives recombination coefficients by interpolating on a table that lives in the data directory. This command tells the code to compute recombination coefficients on the fly by integrating over the photoionization cross section.

10.8.11. atom He-like redistribution [options]

The keyword **redistribution** will change the form of the redistribution function for various lines within the model atom.

A keyword to specify which set of lines to change is required. This is one of **alpha** (the 2 ^1P – 1 ^1S transition), **resonance** (any higher Lyman line decaying to the ground term), or **subordinate** (all Balmer, Paschen, etc lines). The type of redistribution function to use must also be specified. The options are **_PRD** (partial redistribution), **_CRD** (complete redistribution with Doppler core only), and **CRDW** (complete redistribution with damping wings). (The underscore indicates a space.)

The keyword **show** tells the code to print the current default redistribution functions.

10.9. Case B [tau ly alpha = 9; options]

This command is used to check the line emission from the hydrogen and helium atoms in the Case B limit (AGN3 section 4.2). This command *should not* be used in any model that is supposed to represent a real physical environment. It is intended only to provide an easy way to check predictions of the code against simple, more limited, calculations. In particular, when this is used the Lyman-line optical depths will be made artificially large. This may affect the ionization and temperature of the gas.

With no options this command sets the inner optical depth of Lα for all atoms and ions of the H- and He-like iso-electronic sequences to 10^5 so that even a one-zone model will be close to Case B[22]. The optional number is the log of the Lα optical depth. One-sided escape probabilities are used so the total escape probability is simply that for the inward direction. In keeping with the Case B approximation the **Case B** command suppresses excited states line optical depths.

The atoms include all collisional processes. Case B does not define the population of the ground or first excited state so a true comparison with Case B results should have collisions from these levels turned off. This is done with the Hummer and Storey option (with the key **humm**), to allow comparison with their 1987 and 1995 papers. Collisions from the ground and first excited states *are* included if this second option is not specified. Collisions between levels with $n \geq 3$ *are* included unless the **atom H-like collision off** or **atom He-like collision off** commands are given. Collisions between the 2*s* and 2*p* states are always included unless the **atom H-like collisions 2s2p off** command is given.

In the case of the He-like isoelectronic sequence the **Case B** command sets the optical depths in the singlet Lyman lines to a large value. The Hummer & Storey option has no effect on the He-like sequence.

The **no Pdest** option turns off destruction of Lyman lines by background opacity.

There are several side effects of this command that may after the spectrum or physical conditions in unexpected ways. The large Lα optical depth will often result in an especially strong radiation field within this line. This affects the gas through photoionization of excited metastable states of H and He and of those elements with a small enough ionization potential. The **no photoionization** option on the **Case B** command tells the code not to include photoionization from excited metastable states like the 2*s* level of H^0. But these strong diffuse fields will also strongly affect the level of ionization of the gas, making the resulting ionization equilibrium a fiction. Optically thin gas is actually described by Case C (Ferland 1999 AGN3 Section 11.4) where continuum pumping enhances Balmer lines. The large Lyman line optical depths that result from the **Case B** command will prevent continuum resonant pumping of the atom. Beware.

This command is used in the test suite to perform classical PDR simulations which ignore the H II region and assume that the PDR is illuminated by a radiation field with no hydrogen-ionizing radiation. Classical PDR calculations do not include a full treatment of H or He so their ions are only produced by cosmic rays. Cloudy does a full treatment of the physics of H^0 and He^0 and will find a thin layer of highly ionized gas. This is produced by Lyman line pumping into excited states, especially

[22] Before version 96 the default optical depth was 10^9. This caused extreme Lα behavior in a grain-free H II region. The lower value is a better estimate of the physics that occurs in an actual H II region.

metastable 2*s*, which are then photoionized by relatively low-energy light. The process stops when the Lyman line optical depths become large enough for the atom to become self-shielding. The **`Case B`** command will stop this process from ever becoming important by starting with large Lyman line optical depths. (The process would not happen in a realistic calculation which included the H^+ region since Lyman line optical depths through the H^+ region are large.)

This command is included in the PDR simulations in the test suite to stop Lyman line pumping from occurring. A better solution would be to include the PDR as a additional layer outside the H II region. The Lyman line optical depths across the ionized gas will be large and prevent continuum pumping from occurring in the PDR. Combining the H II region and PDR also results in a self-consistent calculation (Abel et al. 2005).

10.10. diffuse fields [outward, ots]

This specifies which method is to be used to transfer the diffuse fields, the emission from gas within the computed structure. The options are **`outward only`** and **`_ots`**.

The **`_ots`** option takes into account optical depths in both the inward and outward directions. The **`_ots`** option has a **`SIMPLE`** option which will do a very simple OTS approximation without taking optical depths into account. All diffuse fields with energies capable of ionizing hydrogen are assumed to do so, and those with smaller energies freely escape. This is a debugging option.

If **`outward`** is chosen then the code will check for a number. This determines which of the many forms of the outward-only approximation (Tarter 1967) is used. The default[23] is 2. This is intended for testing the code.

This choice does not strongly affect the predicted emission-line spectrum, but it does change the temperature at the illuminated face of the cloud. These approximations are described in Part 2 of this document.

10.11. double optical depths

On second and later iterations the code uses the total optical depths of the computed structure to find the outwardly-directed radiation field. This command doubles the total optical depth so that the shielded face of the cloud becomes the mid-plane of a structure that is twice as thick as the computed cloud.

This original purpose of this command was to simulate a geometry in which ionizing radiation strikes the plane-parallel cloud from both sides. Examples are a Lα forest cloud or the diffuse ISM. The total line and continuum optical depths are set to twice the computed optical depth at the end of the iteration. The computed model is then one half of the cloud and the other half of the cloud is assumed to be a mirror image of the first half. Doubling the total line and continuum optical depths

[23] OTS was the default in version 86 and before.

at the end of the iteration is the *only* effect of this command. Physical quantities such as the physical thickness, column densities, or line emission *are not* affected.

This approximation makes sense if the cloud is optically thick in lines but optically thin (or nearly so) in continua. Lines such as the Lα transitions of He I and He II can be important sources of ionizing radiation. Their transport will be handled correctly in this limit when this command is used. Continuum transport out of the cloud will also be treated correctly, but attenuation of the incident continuum will *not* be if the cloud is optically thick in the continuum.

The second use of this command is when the outer edge of a computed structure is not the other edge of the cloud. A typical PDR calculation is an example. The calculation starts at the illuminated face and continues until the gas becomes cool and molecular. The stopping point often does not correspond to the outer boundary of the molecular cloud, but rather is a point that is "deep enough" for a given study. The optical depths are always computed self-consistently. On second and later iterations the total optical depths are normally those of the computed structure. Near the shielded face the outward optical depths will be small and radiation will freely escape in the outward direction. The gas temperature may fall dramatically due to the enhanced cooling resulting from the free escape of line photons. In real PDRs considerable neutral or molecular material probably extends beyond the stopping point so that line photons do not freely escape. The shielding effects of this unmodeled extra material can be included with this command. Then, the shielded face of the cloud will correspond to the mid-plane of the overall structure and lines will not artificially radiate freely into the outer (unmodeled) hemisphere.

10.12. iterate [2 times]

This specifies the number of iterations to be performed. The default is a single iteration, a single pass through the model. At least a second iteration should be performed in order to establish the correct total optical depth scale when line transfer or radiation pressure is important. Two iterations are sometimes sufficient and will be done if no numbers are entered on the command line. A comment will be printed after the last iteration if the total optical depth scale has not converged and further iterations are needed.

10.12.1. Number of iterations

There is a slight inconsistency in how the code counts the number of iterations. The way it functions in practice is what makes the most sense to me.

The word *iterate* is from Latin for "again". So the true number of "agains" should be one less than the total number of calculations of the cloud structure. When the **iterate** command is not entered there is one calculation of the structure and so formally no iterations. If any one of the following commands is entered:

```
iterate
iterate 0
iterate 1
iterate 2
```

then exactly two calculations of the structure will be done. If the number on the line is two or greater, then the number will be the total number of calculations of the structure.

10.12.2. iterate to convergence [max =7, error =.05]

This is a special form of the **`iterate`** command in which the code will continue to iterate until the optical depths have converged or a limit to the number of iterations has been reached. The optional first number on the line is the maximum number of iterations to perform with a default of 10. The second optional number is the convergence criterion. The default is for relative optical depths to have changed by less than 0.20 between the last two iterations. The optional numbers may be omitted from right to left. If all transitions are optically thin then only a second iteration is performed.

10.12.3. Convergence problems

The code generally will not converge if it has not done so within ten or so iterations. The most common reason for convergence problems is that the specified column density or thickness causes the simulation to end very near a prominent ionization front. In this case very small changes in the physical conditions result in large changes in the optical depths. This is a physical, not numerical, problem. The code will not have convergence problems if an optical depth is used as a stopping criterion instead.

10.13. no scattering opacity

This turns off several pure scattering opacities. These include scattering by grains, electron scattering, and the extreme damping wings of Lyman lines (Rayleigh scattering). When scattering opacity is included and an open geometry is computed the scattering opacity is assumed to attenuate the incident radiation field as $\left(1+0.5\tau_{scat}\right)^{-1}$ rather than $\exp\left(-\tau\right)$ (Schuster 1905).

Scattering can be neglected in a spherical geometry with gas fully covering the source of ionizing radiation. Scattered photons are not really lost but continue to diffuse out with (perhaps) a slight shift in energy. Electron scattering is generally the most important scattering opacity in a grain-free mixture. If $\tau_{scat} \le 1$ then it is reasonable to consider electron scattering as a heating and cooling process but not as an absorption mechanism if the energy shifts are not large (i.e., $h\nu ?\ \ mc^2$) and the geometry is spherical (this is not correct for γ-ray energies, of course). Cloudy is not now designed to work in environments that are quite Compton thick, but should work well for clouds where the electron scattering optical depths are less than or of order unity. When this command is entered Compton energy exchange and recoil ionization are still included as heating, cooling, and ionization processes, but not as opacity sources. (Thermal and ionization effects of Compton scattering are turned off with the **`no Compton`** command described on page 201 below). The **`no scattering opacity`** command is automatically generated when **`sphere`** is specified.

10.14. turbulence = 100 km/sec [_log, dissipate]

This enters a microturbulent velocity u_{turb}. The velocity is given in km s^{-1} on the command line although the code works with cm s^{-1} internally. If the optional keyword **_log** appears then the number is interpreted as the log of the turbulence.

Turbulent pressure is included in the equation of state when the total pressure is kept constant (see page 69 above)[24]. The **no pressure** option on this command says not to include turbulent pressure in the total pressure.

Turbulence affects the shielding and pumping of lines. Fluorescent excitation of lines becomes increasingly important for larger turbulent line widths since a larger part of the continuum can be absorbed by a line. Line pumping is included as a general excitation mechanism for all lines using the formalism outlined by Ferland (1992) and described further in a section of Part 2. The line-center optical depth varies inversely with the line width velocity u so the effects of line optical depths and trapping become smaller with increasing line width. Larger u inhibits self-shielding.

10.14.1. Definitions

The Doppler width of any line that is broadened by both thermal motions and turbulence that is given by a Gaussian is given by the quadratic sums of the thermal and turbulent parts,

$$u = \sqrt{u_{th}^2 + u_{turb}^2} = b = \sqrt{2}\sigma \ \ [\text{cm s}^{-1}] \ . \qquad (50)$$

Here b is the Doppler parameter used in much of the UV absorption-line literature, σ is the standard deviation (often called the dispersion) for a normal distribution, and σ^2 is the variance. For a thermal distribution of motions the average velocity along the line of sight (Mihalas 1970, equation 9-35, page 250) and the most probable speed (Novotny 1973, p 122) of a particle with mass m are both given by

$$u_{th} = \sqrt{2kT/m} \ \ [\text{cm s}^{-1}] \ . \qquad (51)$$

The turbulent line width u_{turb} is zero by default. This command sets u_{turb}. Note that with these definitions the full-width half-maximum (FWHM) of a line is equal to

$$u(FWHM) = u\sqrt{4\ln 2} \ \ [\text{cm s}^{-1}] \ . \qquad (52)$$

10.14.2. Turbulent pressure

For an ideal gas the thermal pressure is $P = nkT$ while the energy density is $1/2\,nkT$ per degree of freedom, so for a monatomic gas is $U = 3/2\,nkT$. Turbulent motions add pressure and energy terms that are analogous to thermal motions if the turbulence has a Gaussian distribution. Note that the turbulent velocities may be organized, or lined up in certain directions, if the gas is magnetically controlled. This presents a complication that is ignored.

[24] Turbulence was not included as a pressure term in versions 06.02 and before.

Heiles & Troland (2005) discuss both turbulence and magnetic fields. Their equation 34 gives the turbulent energy density in terms of the one-dimensional turbulent velocity dispersion $\Delta V_{turb,1D}^2$ (or standard deviation). Note that we write velocities in terms of u with the relationship $u^2 = 2\Delta V_{turb,1D}^2$. Their energy density can be rewritten as a pressure:

$$\begin{aligned} P_{turb} &= \frac{F}{6}\rho u_{turb}^2 = 3.9\times 10^{-10} F\left(\frac{n_{tot}}{10^5\ \mathrm{cm}^{-3}}\right)\left(\frac{u_{turb}}{1\ \mathrm{km\ s}^{-1}}\right)^2 \quad \left[\mathrm{erg\ cm}^{-3};\ \mathrm{dynes\ cm}^{-2}\right] \\ &= 2.8\times 10^{6}\ F\left(\frac{n_{tot}}{10^5\ \mathrm{cm}^{-3}}\right)\left(\frac{u_{turb}}{1\ \mathrm{km\ s}^{-1}}\right)^2 \quad \left[\mathrm{cm}^{-3}\ \mathrm{K}\right] \end{aligned} \tag{53}$$

where n_{tot} is the total hydrogen density, u_{turb} is the turbulent velocity, and He/H = 0.1 was assumed. The term F accounts for how the turbulent velocity field is ordered. (Heiles & Troland 2005, their equation 34). F is 2 for turbulent velocities that are perpendicular to the magnetic field as in Alfven waves and F is 3 for isotropic turbulent motions. The default value of F = 3 is changed by entering a new value as a second number on this command line.

10.14.3. Equipartition turbulent – magnetic pressures

The **`equipartition`** option on the **`turbulence`** command sets the turbulent velocity to an equipartition between magnetic and turbulent energy densities. That is,

$$P_{turb} = \frac{F}{6}\rho u_{turb}^2 = P_{mag} = \frac{B^2}{8\pi} \ [\mathrm{erg\ cm}^{-3}]. \tag{54}$$

The **`magnetic field`** command (page 109 below) sets B. The turbulent velocity is determined from the magnetic field assuming equation 54. Heiles & Crutcher (2005) argue that the correlation between turbulent and magnetic pressures, while true on average, does not hold in detail for specific regions of the ISM.

10.14.4. Energy dissipation

The **`dissipate`** option on the **`turbulence`** command provides a way in include conversion of wave energy into heat (see Bottorff & Ferland 2002). When the option is used a third number, the log of the scale length for the dissipation in cm, must appear. Then the turbulent velocity will have the form

$$u_{turb}(r) = u_{turb}(r_{\mathrm{o}})\exp(-\Delta r / r_{scale}) \quad [\mathrm{cm\ s}^{-1}] \tag{55}$$

where $u_{turb}(r_{\mathrm{o}})$ is the turbulence at the illuminated face and Δr is the depth into the cloud. The wave mechanical energy is assumed to have been converted into heat with a local heating rate given by (Bottorff & Ferland 2002)

$$G(r) = 3.45\times 10^{-28} 2^{-3/2} u_{turb}(r)^3 \quad [\mathrm{erg\ cm}^{-3}\ \mathrm{s}^{-1}] \tag{56}$$

10.14.5. turbulence command heads up!

N.B.! The turbulent velocity is the first number on the command line. The F parameter is the second number. In the equipartition case it is still necessary to specify a turbulent velocity if you also want to specify *F*, since *F* must be the second number. In the equipartition case the specified turbulent velocity is not used for anything, but it must still be there. The energy-dissipation scale length is the third number and must appear after u_{turb} and *F*. These numbers can only be omitted from right to left.

10.15. vlaw x x

This specifies a turbulent velocity that is a power law in radius. The number is the power law on radius. It must be negative.

11. THERMAL SOLUTIONS

11.1. Overview

This section describes options that affect the thermal solution and the gas kinetic temperature.

The accuracy of the thermal solution is set by the error tolerance in the heating – cooling balance. This is set with the **`set temperature tolerance`** command described on page 219 below. It also can be used to change some details of the thermal solution. The error tolerances in other quantities are described on page 205 below.

11.2. cextra -14.231 [temp to the 1.5 power]

This adds an extra cooling term due to some unspecified physical process. The first number is the log of the cooling rate [erg cm^{-3} s^{-1}]. The second number is an optional exponent that specifies a temperature dependence. The cooling will be given by

$$\Lambda = 10^{c_1} \times \left(\frac{T_e}{10^4\ \mathrm{K}} \right)^{c_2} \ [\mathrm{erg\ cm^{-3}\ s^{-1}}] \qquad (57)$$

where c_1 and c_2 are the two numbers entered with this command. If the second optional argument c_2 is not specified then zero (i.e., constant cooling) is assumed.

The function evaluating cextra is given by the variable ***cextxx***. The expression can be easily changed to other forms by changing how this variable is set.

11.3. constant temperature, t=10,000K [linear]

A constant electron temperature calculation will be performed. The number is either the electron temperature itself but is interpreted as the log of the temperature if ≤ 10. The optional keyword **`linear`** forces that interpretation. The temperature must be within the temperature limits of the code, currently 2.8 K < T < 10^{10} K.

By default the temperature is specified in Kelvin. The keywords **`_eV_`** and **`_keV`** are also accepted.

Collisional ionization of all atoms and ions is included so this option can be used to produce clouds in coronal or collisional equilibrium.

WARNING! It is also necessary to specify a stopping criterion of some kind when this command is used. Most thermal-equilibrium calculations stop when the electron temperature falls below some lowest value, set with the **`stop temperature`** command (page 126 below) and with the default value 4000 K. This cannot happen with a constant-temperature model. For instance, a constant temperature model of a planetary nebula will continue until the default limit to the number of zones (now 1400) is reached. The *vast* majority of the cloud will consist of predominantly neutral gas well outside the hydrogen Strömgren sphere. This gas will have a small ambient level of ionization and emission due to collisional ionization. The resulting emission-line spectrum might be surprising since the neutral gas contributes significant emission.

Any of the stopping criteria described in the Chapter *Stopping Criteria,* starting on page 119 below, can be used. A more physical constant temperature model of a ionized cloud could be done by using the **`stop efrac`** (page 123 below) command to stop the calculation when the hydrogen ionization front is reached.

11.4. constant grain temperature 20K [linear]

Normally the temperature of each grain material and size is determined by balancing heating and cooling. This command sets the grain temperature to the indicated quantity.

If the **`linear`** keyword appears then the number is always interpreted as the linear temperature. Otherwise numbers ≤ 10 are interpreted as a log of the temperature.

Other aspects of the grain physics are controlled with the **`grain`** command, described on page 58 above.

11.5. coronal equilibrium, T=10,000,000K [linear]

Coronal equilibrium, in which the gas is collisionally ionized, is assumed. The number is interpreted as the log of the temperature if the argument is ≤ 10 and the linear temperature otherwise. The optional keyword **`linear`** will force the interpretation as the linear temperature. This holds the electron temperature at the specified value.

It is necessary[25] to also specify some sort of stopping criteria. The calculation will probably continue until the default limit to the number of zones is reached if a stopping criterion is not specified.

Figure 9 shows the soft X-ray line and continuum emission predicted from the input stream in the test case **`ism_hot_brems.in`**.

The **`time init`** option provides a way to set initial conditions for a time-dependent cloud. See the description of the **`time`** command, on page 112 below, for further details.

11.6. cosmic rays [options ….]

This adds cosmic ray and their heating and ionization. This physics is described by Ferland & Mushotzky (1984), the subsection *Cosmic Ray Interactions* in the section *Other Physical Processes* in Part 2 of this document, and section 11.3 of AGN3. Cosmic rays mainly heat ionized gas and both heat and create secondary ionizations in neutral gas. All of this is done self-consistently.

[25] In versions 87 and before, the **`coronal`** command set the zone thickness to 1 cm, and stopped after computing one zone.

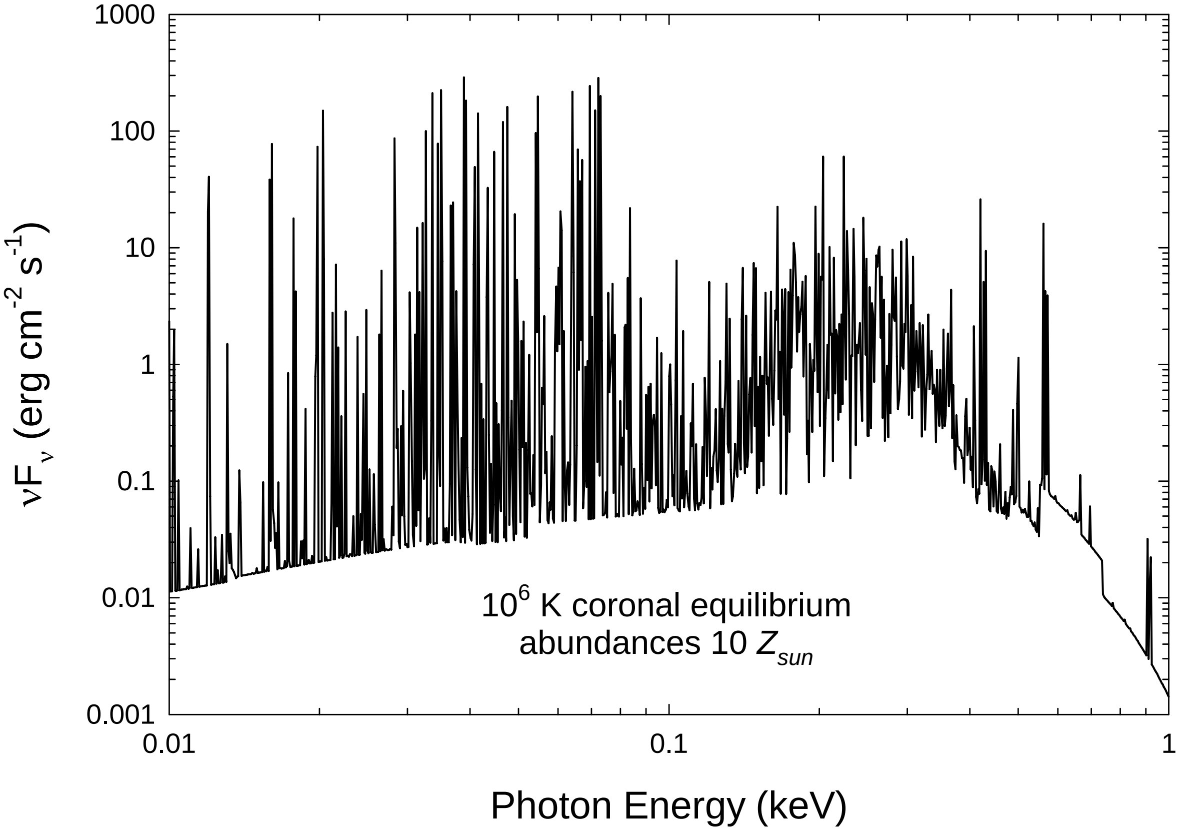


Figure 9 This shows the soft X-ray emission from a simple model of the hot phase of a metal-rich ISM. The input script ism_hot_brems.in was used to create the predicted spectrum.

The **set csupra** command (page 210 below) provides a way to specify a secondary ionization rate. This has many of the same effects as introducing cosmic rays, and uses the same code variables. The rate introduced by the **set csupra** command is not self-consistent with the rest of the calculation but does provide a way to test the code in certain simple limits.

Cosmic rays must be included if the calculation extends into molecular regions. The ion-molecule chemistry that occurs in the cold ISM requires a source of ionization (Dyson & Williams 1997). In fact, most estimates of the galactic cosmic ray background are based on the abundances of chemical ions such as H_3^+ (McCall et al. 2003; Shaw et al. 2008). The chemistry network will probably collapse if the gas becomes molecular but cosmic rays are not present. The code will complain but try to compute the model if a simulation without cosmic rays extends into cold gas. If cosmic rays are not included in the calculation and the neutral hydrogen ionization rate falls below 10^{-17} s^{-1}, the code will print a comment stating that the ionization rate fell below the galactic background rate.

11.6.1. cosmic rays background [1.2]

This includes galactic background cosmic rays. They produce an H^0 ionization rate of 2.5×10^{-17} s^{-1}, an H_2 ionization rate of 5.0×10^{-17} s^{-1} in predominantly neutral gas[26], and a heating rate in fully ionized gas of 2.3×10^{-27} erg s^{-1}. These are based on the cosmic-ray galactic background deduced by Williams et al. (1998). Cloudy determines the heating and ionization rates of cosmic rays self consistently, as appropriate for the local molecular, atomic, and electron densities (see AGN3 Section 11.3).

An optional scale factor specifies the cosmic ray ionization rate relative to this background value. The scale factor is assumed to be a log unless the keyword **`linear`** also appears.

For reference, the study of the starburst in M82 by Suchkov, Allen, & Heckman (1993) find cosmic ray ionization rates that are several dex larger than the galactic background. The background rate is an open question. McCall et al. (2003) find a background rate 1.2 × 10^{-15} s^{-1} for a galactic sight line. This is about 48 times larger than our default. Indriolo et al. (2007) find a mean cosmic ray ionization rate for twenty sight lines through the local ISM of 2×10^{-16} s^{-1}, about ten times higher than our default. Shaw et al. (2008) find a rate forty times larger from detailed modeling of the sight line to Zeta Per. Pellegrini et al (2007) find cosmic ray ionization rate significantly enhanced above the galactic background in M17. This is clearly an area of active research.

11.6.2. cosmic ray rate -17.3

If the keyword **`rate`** appears then the command specifies the log of the H^0 ionization rate [s^{-1}] in predominantly neutral gas. The default is 2.5×10^{-17} s^{-1} taken from Williams et al. (1998).

11.6.3. cosmic rays density =1.2 [index, etc.]

If the keyword **`density`** appears then the first number is the log of the cosmic ray density $n(cr)$ [cm^{-3}]. Expressions given in Ferland & Mushotzky (1984) convert this into an ionization rate.

The second optional number is a power-law index α that describes the variation of the cosmic ray density with radius, i.e.,

$$n(cr,r) = n(cr,r_o)\left(\frac{r}{r_o}\right)^{\alpha} \ [\mathrm{cm}^{-3}] \ . \qquad (58)$$

The default value of the index is α =0, corresponding to a constant cosmic ray density. The third optional number is the log of the temperature of the fast electrons, if they are not relativistic. If this third number is specified then expressions from Balbus and McKee (1982) will be used to evaluate the electron heating rates. The options can be omitted from right to left.

[26] Before 2004 the code used a background ionization rate of 7.4×10^{-18} s^{-1} quoted by Tielens and Hollenbach (1985a; Table 10) and McKee (1999).

11.6.4. cosmic ray equipartition

The cosmic rays are assumed to be in equipartition with the magnetic field. Then the cosmic-ray density is given by

$$n(cr,B) = n(cr,B_0)\left(\frac{U(B)}{U(B_0)}\right) \text{ [cm}^{-3}\text{]} \qquad (59)$$

where $U(B)$ and $U(B_0)$ are the energy densities of the local magnetic field relative to the galactic background magnetic field. The **magnetic field** command (page 109 below) sets B. Webber (1998) gives a cosmic-ray energy density of 1.8 eV cm^{-3}, which corresponds to a magnetic field of 8.5 μG if equipartition holds. The background cosmic-ray ionization rate is scaled by the ratio of the magnetic energy densities to find a local cosmic ray ionization rate and energy density.

11.7. failures 100 times [map]

A converge failure occurs when the heating-cooling balance, the electron density, or the pressure, is not within the tolerance set by the **set convergence** commands (page 205 below). Normally Cloudy will punt[27] after an excessive number of convergence failures (presently 20) occur. This command increases the number of allowed failures to the value entered as a parameter.

When Cloudy stops because of excessive failures and the **map** option is specified[28] as a keyword on the **failures** command it first produces a map of (heating-cooling) versus temperature to give an indication of where the equilibrium temperature should have been. A section in Part 3 describes thermal failures in more detail and describes this output.

Failures most often occur near a thermal front. This occurs when the solution jumps over peaks in the cooling function that occur near ~2000 K and ~10^5 K. A warning will be issued at the end of the calculation if the global thermal balance is wrong.

It should not be necessary to use this command. Please post the example on the discussion board if you find a simulation where you need to increase the number of convergence failures.

11.8. force temperature to 3400K

This forces the initial estimate of the temperature of the first zone to the value entered. The temperature is interpreted as a log if it is ≤ 10 and the linear temperature otherwise. The keywords **_log** and **linear** will override this.

[27] FAQ: Punt is a technical term from American football. It is something bad that happens when progress in advancing the ball is lacking.

[28] In versions 94 and before, the default was to produce the map, and the **no map** option turned this off. With version 95 the option is not to produce a map, and this must be requested with the **map** option.

This command is useful if more than one initial temperature solution is possible. It forces the first guess of the temperature to the specified value but *does not* hold the temperature constant. The temperature is determined by energy balance thereafter. (A constant kinetic temperature is set with the **`constant temperature`** command.)

Cloudy may have trouble finding a valid first temperature if the initial solution is forced well away from the equilibrium value. This is an inevitable consequence of the complete linearization methods that are intrinsic to the code's solvers. If a large number of thermal failures or warnings result from the use of this command then it is likely that the code has been forced too far away from the solution. A better guess of the initial temperature would fix this problem.

11.9. hextra -14 [depth, density, time]

This includes extra heating due to some unspecified energy source. The first number H_0 is the log of the volume-heating rate [erg cm^{-3} s^{-1}]. Optional keywords specify how this heating depends on density, depth into the cloud, or time. If these optional keywords do not occur then the heating is constant.

11.9.1. hextra -14 depth 18, thickness 12

The keyword **`depth`** makes the heating vary with depth into the cloud. The second number is the log of the scale radius r_{scale} [cm]. The extra heating rate varies as[29]

$$H = H_0[\exp(-depth / r_{scale}) + \exp(T - depth) / r_{scale})] \text{ [erg cm}^{-3}\text{ s}^{-1}\text{]}. \qquad (60)$$

The third optional parameter T is the total thickness of the slab. If this is given then the second exponential term will be added. This will mimic an external heat source that warms the cloud from both the illuminated and shielded faces. If the third parameter is not entered then the rightmost term is not included.

11.9.2. hextra -13 density

The **`density`** option makes the heating scale with the hydrogen density. The heating will be given by

$$H = H_0\left[n(H) / n_0\right] \text{ [erg cm}^{-3}\text{ s}^{-1}\text{]}. \qquad (61)$$

where n(H) is the local hydrogen density [cm^{-3}] and n_0 is a scale density. The scale density is unity by default and is changed by specifying the optional second number, the log of the scale density.

11.9.3. hextra time

If the **`time`** keyword appears then the variable scale factors that appear on the **`time`** command (page 112 below) will multiply the heating rate specified with the **`hextra`** command. This makes it possible to follow the effects of time-dependent heating sources.

[29] In versions through 94.00 the heating rate varied as $exp[-r_{scale}/(r-r_o)]$ and went to infinity as the illuminated face. The radial dependence was changed to its current form in 94.01.

11.9.4. Notes on then hextra command

The heating can only depend on depth or density but the **`time`** option can also be specified for each.

By default a calculation will stop when the kinetic temperature falls below 4000 K. It will be necessary to set other stopping criteria such as the cloud thickness if the extra heating keeps the gas warmer than this limit.

11.10. high temperature approach

This command tells the code to search for the first temperature by approaching the thermal solution from the high temperature extreme of 10^6 K. Normally the approach is from low temperatures. This can be useful when more than one thermal solution is possible.

11.11. magnetic field, log(B) = 5 [options]

Magnetic fields are not included by default. This specifies the strength and geometry of the magnetic field. A number, the log of the magnetic field strength in Gauss, is the first number on the line. The physical effects of magnetic fields are discussed in Part 2 of this document.

Ordered and tangled fields can be specified. The field is assumed to be tangled by default. If the keyword **`ordered`** appears then the angle between the radiation field of the central object and the magnetic field is also specified. This angle is zero if the field is in the outward radial direction. The angle is given in degrees by default but the **`radian`** keyword will cause it to be radians instead.

In the case of a tangled field the code will look for a second number, the index for the gamma-law relation between the magnetic field and the gas density. If a second number is not found then an index of $\gamma = 4/3$, appropriate for a tangled field, will be assumed. This index appears in the relationship

$$B_{\rm tangled} = B_{\rm tangled}^{0} \left(\frac{\rho}{\rho_0} \right)^{\gamma/2} \ [\text{Gauss}] \qquad (62)$$

where the term in parenthesis is the ratio of the current density to the density at the illuminated face of the cloud. For a spherical constant-velocity flow, where $\rho/\rho_0 \propto (r/r_0)^{-2}$, the field will vary as $B/B_0 \propto (r/r_0)^{-\gamma}$. This is in contrast with a dipolar field, in which the radial dependence is $B/B_0 \propto (r/r_0)^{-3}$.

Both ordered and tangled fields can be specified on separate commands. If more than one ordered or tangled field is specified then the second will take precedence over the first.

The major thermal effect of a field is to add cyclotron cooling. This is only important at very high temperatures.

Magnetic pressure and enthalpy terms corresponding to the magnetic energy density are included in the equation of state when a constant-pressure geometry is assumed. The magnetic pressure is

$$P_B / k \approx \frac{B^2}{8\pi k} \approx B_{100\mu G}^2 2.9 \times 10^6 \ \ [\mathrm{cm}^{-3}\ \mathrm{K}] \qquad (63)$$

where $B_{100\mu G}$ the magnetic field in units of 100 μG. The plasma β parameter, defined as the local ratio of thermal to magnetic energy densities, $\beta = P_{gas} / P_{mag}$, is printed in the summary of pressure contributions. The field affects the dynamics of the gas when $\beta \le 1$.

Supersonic turbulence in rough energy equipartition with the magnetic field is often observed in the cold ISM (Heiles & Crutcher 2005). The **`turbulence`** command (page 100 above) has an **`equipartition`** option to set the turbulent velocity to a value in energy equipartition with the magnetic field. Although a general correlation is observed in the cold neutral medium of the ISM, it is not thought to be a fundamental relationship (see the Heiles & Crutcher paper).

11.12. map, zone 4 [range 2000, 5000]

This computes the heating-cooling vs temperature relation (a "thermal map") of the zone specified as the first number on the line. This is one way to check for the existence of more than one thermal solution. If no zone is specified, or if the zone is less than or equal to 0, then only a thermal map is produced for the illuminated face of the cloud and the calculation then stops. The calculation of the heating and cooling is self-consistent across this map. A section in ***Problems*** in Part 3 of this document explains how to interpret the map output.

The map produced by this command is not directly comparable to the more typical plot that shows the equilibrium temperature as a function of ionization parameter (Krolik, McKee, and Tarter 1981). That map can be produced by successively calling Cloudy with the same ionizing continuum but different densities, say, with the **`grid`** command (page 199 below). In that second case each deduced temperature is a valid equilibrium temperature. In the map produced by the **`map`** command only one temperature, where heating and cooling are equal, is a valid equilibrium temperature. The map produced by this command is useful for checking for more than one thermal solution, to check that the heating and cooling curves smoothly flow as the temperature changes, or to investigate why the code had convergence problems (it was originally introduced for only this latter purpose).

The optional keyword **`range`** specifies the temperature range of the map. If this option is specified then the first number on the line must be the zone for the map, zero if only a map of the first zone, and the next two numbers must be the lower and upper limits to the map. These temperatures will be interpreted as logs if the first temperature is ≤ 10. Normally about 20 steps occur between the lowest and highest temperature in the map. The number of steps can be reset with the **`set nmaps`** command (page 215 below).

The thermal map can be saved as a separate file with the **`punch map`** command (page 165 below). This produces output that is suitable for processing by other software.

The code stops when the map is complete since it is left in a disturbed state.

11.13. neutrons -2 [efficiency =-2]

This adds energy deposition and ionization by secondaries due to the fast neutrons proposed by Sikora, Begelman, and Rudak (1989). The argument is the luminosity in fast neutrons expressed as a fraction of the *total* photon luminosity of the incident continuum. It is interpreted as a log if ≤ 0 and a linear scale factor if positive.

The second optional argument is the heating – ionization efficiency of the neutrons, unity by default. Both quantities are interpreted as logs if ≤ 0 and linear if positive.

11.14. print coolants, zone 135

See page 132 below.

11.15. print heating

See page 133 below.

11.16. set temperature [floor, solver, convergence]

See page 219 below.

11.17. tlaw [DB96, SN99]

This specifies a temperature law. Although code does exist to allow the range of options enjoyed by the **dlaw** command (page 70 above) only two options currently are implemented.

The **DB96** option tells the code to use the temperature – column density law used by Draine & Bertoldi (1996):

$$T = T_0 / \left[1 + N(\mathrm{H})\sigma_{d,1000}\right] \quad [\mathrm{K}] \tag{64}$$

where T_0 is 500 K and σ is 6×10^{-22} cm^2.

The **SN99** option tells the code to use the temperature – H_2 fraction relationship assumed by Sternberg & Neufeld (1999);

$$T = \frac{500}{1 + 9\left[2n(\mathrm{H}_2)/n(\mathrm{H}_{tot})\right]^4} \quad [\mathrm{K}]. \tag{65}$$

12. DYNAMICAL & TIME-DEPENDENT CALCULATIONS

12.1. Overview

This section describes the dynamical and time dependent calculations that can be done with the code. This physics was developed in collaboration with Robin Williams and Will Henney, and Henney et al. (2005) and Henney et al (2007) describe first applications.

These calculations begin by doing several iterations to compute the static structure. This establishes the optical depth scale that is used in later calculations. The number of static calculations is 2 by default and is reset with the **`set dynamics relax`** command described on page 118 below.

Advective terms are included in the balance equations by adding upstream quantities that are taken from the previous iteration. Problems would arise if we needed to look upstream beyond the outer edge of the computed radial grid. To prevent this the outer radius found in the static iterations will be the outer radius of later calculations. This overrides the behavior of the **`radius`** command.

Warning! The physics behind these commands is still being developed. The heuristics that are needed to control changes in the time steps or the advancing upstream parameters are not complete. Output options to capture the information in the flow or over time are not complete. All of this is an area of active development.

☠In the following commands that are still under development are introduced by the skull symbol and are in a grey box.

12.2. ☠time dependent, time step = 7.5, stop at 9.5

This follows the time-dependent evolution of a cloud near a variable continuum or heat source.

Time-dependent calculations are done by setting up an initial geometry using the usual commands that specify a cloud and its continuum source. The **`time`** keyword establishes which energy sources vary with time. The keyword can appear on any of the commands that specify the continuum luminosity and on the **`hextra`** command (page 108 above).

If a **`time`** command also occurs then all luminosity and heat sources with the **`time`** keyword will change with time. The **`time`** command sets a time step and stopping time. Each iteration is a time step and the number of time steps is set with the **`iterate`** command. The calculation will stop when either the number of iterations or the stopping time is reached.

A series of static calculations is first done to insure that we start from a stable solution. The number is 2 by default and is reset with the **`set dynamics relax`** command described on page 118 below. These occur at time 0. The first iteration after these initial solutions will occur at a time given by this time step.

12.2.1. *Constant time steps*

The first numerical argument on the **time** command is the log of the time step in seconds. The second optional argument gives the log of the stopping time in seconds. By default the time step is kept constant. The calculation starts at time zero so the number of iterations will be the ratio of the stopping time to the time step.

The **time** command is followed by a table giving the logs of the elapsed time (seconds) and the log of a scale factor giving the brightness of the variable source relative to its initial value. The code will not extrapolate beyond the end of the table. It will stop if it needs to look up times beyond the last tabulated value. The following is a simple example:

```
// set the continuum and a variable flux of H-ionizing photons
blackbody T=40,000K
phi(H) 13.5 time
// set a limit of 50 time steps.  The calculations will actually
// stop when we reach total age
iterate 50 times
// the time command sets a time step of 1e7 s and a stop time of 1e8 s.
// This requires ten time steps.  We set 50 iterations above but the
// calculation will actually stop when the age of 1e8 s is reached.
// The time command is followed by a table giving the log of the age and the
// log of the brightness of the energy source relative to its initial value.
// The table ends with the line saying “end of times”
time steps=7 s stop at 8 s
age = 0 scale = 0
age = 7.3 scale = 0
age = 7.35 scale = 5
age = 7.5 scale = 5
age = 7.55 scale = 0
age = 10 scale = 0
end of times
// commands to set hydrogen density, only done one zone
hden 5
stop zone 1
```

In this example only one continuum source is given and the flux of hydrogen-ionizing photons varies with time. A constant time step of 10^7 s is used. The time command is followed by the series of lines giving the continuum brightness as a function of time. The series ends with the line starting with **end**. Each of the lines in the age – brightness table starts with **age** but these characters are ignored. They are only present to improve readability.

12.2.2. *Time-step size increment*

```
c first set the continuum
blackbody T=40,000K
c this continuum will vary with time
ionization parameter -2 time
c the CMB will be constant
CMB
c do 50 time steps
iterate 50 times
c the time command itself, followed by a table of times & continua
time 7.5
 7     scale= 0
 7.1   scale=-5 recombination
 9.3   scale=-5
 9.301 scale= 0 ionization, factor = 1.1
 20    scale= 0
end of time
```

```
c first set the continuum
blackbody T=40,000K
c this continuum will vary with time
ionization parameter -2 time
c the CMB will be constant
CMB
c do 50 time steps
iterate 50 times
c the time command itself, followed by a table of times & continua
time 7.5
time = 7     scale= 0
time = 7.1   scale=-5 recombination
time = 9.3   scale=-5
time = 9.301 scale= 0 ionization, factor = 1.1
time = 20    scale= 0
end of time
```

In this example the continuum is a blackbody with its intensity set by an ionization parameter. The code does fifty iterations with a time step of $10^{7.5}$ s since this is specified on the initial **time** command line. In the table the continuum is left at its initial value for the first 10^{7} s then lowered to 10^{-5} of the initial value for a total of $10^{9.3}$ s, when it is raised back to the initial value.

As given above, the time steps always have the same size, the size given on the initial **time** command. It is also possible to specify the size of the time step for each elapsed time that appears in the table that gives the continuum brightness. If all of the optional time-step sizes are specified then they are used in place of the time step given on the **time** command. The time step sizes are multiplicatively increased by the time-step scale factor. It is also possible to give a time-step scale factor saying how to increase the time step.

If any are missing then the time step on the command is used and is kept constant. The table ends with a line saying **end_**. If the optional end time is not specified on the **time** command then the calculation will continue until the specified number of iterations has been performed.

12.2.3. Keywords on individual time-step entries

Most of the letters on the lines giving the times and scale factors are totally ignored. They are there to make the table easier to read. There are keywords which indicate that a particular time step marks the start of a special case, such as the recombination of a highly ionized gas or the propagation of an ionization front into neutral gas.

The keyword **recombination** indicates that this time step is the first where the continuum source will be dramatically fainter. Certain heuristics are used to follow the recombination and cooling of the gas.

The recombination and ionization heuristics are not complete.

12.2.4. Varying individual continua

The keyword **time** is used to specify which continua will be scaled with time and can appear on any of the luminosity / intensity commands given in this chapter. This makes it possible to vary only some of the continua while others are left constant. For instance, a constant CMB and a variable star can be treated. At least one of the luminosity commands must have a **time** keyword for time-dependent calculations to be done.

The **hextra** command (page 108 above) includes the **time** keyword. The variable scale factor will apply to the extra heating in this case.

12.2.5. Other commands

The **coronal** command, describe on page 104 above, has the **time init** option. This will include thermal collisional ionization for the initial evaluations of the simulation. The electron temperature will be free when the time-dependent calculation starts.

12.2.6. Output options appropriate for time command

Punch commands work as expected, with every time step counting as an iteration. If you the **last** option you will only obtain punch output for the last time step.

12.3. wind u=300 km/sec [mass =1.4 Msun, disk]

The envelope is a wind. The first number is the initial velocity in km s^{-1}. The second optional number is the central mass in solar mass units. Both are linear quantities.

The equations of motion are solved including the inward pull of gravity. The gravitational acceleration in the default non-rotating case is evaluated as

$$g = -\frac{GM}{r^2} \quad [\mathrm{cm\ s^{-1}}]\ . \qquad (66)$$

The mass of the central object is given in solar masses on the command line but is evaluated in gm within the code. If the mass is not specified then zero is assumed. If the mass is specified and the keyword **disk** also appears then the geometry is assumed to be a rotating disk. In this case the inward gravitational acceleration is

$$g = -\frac{GM}{r^2}\left(1 - \frac{r_o}{r}\right) \quad [\mathrm{cm\ s^{-2}}] \qquad (67)$$

where r_o is the inner radius.

The line widths and escape probabilities are evaluated in the Sobolev or Large Velocity Gradient (LVG) approximation. The effective line optical depth is given by

$$\tau_{l,u}(R) = \alpha_{l,u} \min(r, \Delta r)\left(n_l - n_u \frac{g_l}{g_u}\right)\left(\frac{u_{th}}{\max(u_{th}, u_{\exp})}\right) \quad [\mathrm{Napier}] \qquad (68)$$

where u_{th} and u_{exp} are the thermal and expansion velocities respectively and the radius used is the smaller of the depth or the radius. This is necessary to keep the effective column density from becoming larger than the total cloud column density when the radius is large and the expansion velocity is small.

12.3.1. *The sign of the velocity*

A *positive velocity* indicates the hypersonic wind solution that has been a part of the code since its beginnings. The equations of motion of the gas are solved. Acceleration due to line and continuous opacity of the gas and deceleration due to the gravity of the central object are included. The calculation will stop if the gas comes to rest or if any of the other stopping criteria is met. The initial velocity must be above the sonic point. Further details are presented in a section in Part 2.

The first parameter is the expansion velocity u_o at the illuminated face of the cloud. The approximations used are only correct if the model begins above the sonic point. The initial velocity must be greater than zero and is entered in km s^{-1}. The density at the illuminated face of the cloud is entered with the **hden** command and the density is varied across the model to conserve mass flux (i.e., the product $\rho(r)r^2 u(r)$ is kept constant). Because of this a filling factor would not make physical sense and should not be used (although it can be). The optional second parameter is the mass of the central star in solar units; its default value is one solar mass.

A *negative velocity* simulates the flow from a weak-D or D-critical H II region (Henney et al. 2005). This physics is currently under development in collaboration with Will Henney and Robin Williams. The central object mass is set to zero.

12.3.2. ☠*wind advection, velocity=-5 km/s*

The **advection** keyword says to include the effects of advection on the thermal and ionization equations. Currently advection is only treated in the case where the velocity is negative, corresponding to a flow off a molecular cloud towards the source of ionizing radiation. The argument is the initial gas flow speed in km s^{-1}. This physics is being developed in collaboration with Robin Williams and Will Henney and is not yet mature.

The advection case has the following options. In all cases the numerical parameter follows the keyword. There can be many parameters on one command line.

velocity – the number following this keyword is the velocity in km s^{-1}. The following would specify a simple *R*-type front

```
wind advection velocity -100
```

center, **index** – A varying mass flux with depth into the grid is specified by a law $\rho u = \Phi_o (r-c)^i$. This gives the variation in flux with distance *r* into the grid as a function of value *c* given by the **center** parameter and the value *i* given by the **index** parameter. For example,

```
wind advection velocity -20 center 10,000,000,000,000,000 index -2
```

would correspond to a wind diverging spherically from a point 10^{16} cm into the grid with a velocity of 20 km s^{-1} at the illuminated face. By default, the mass flux is constant (i = 0). If these are not specified then zero is assumed.

dfdr – This specifies the mass flux gradient, $\Phi' = d\ \rho u / dr$ [g cm^{-3} s^{-1}], as an alternative to specifying the velocity. This is useful in the case in which the flow reaches stagnation at the surface of the model, in which case the velocity itself does not fully constrain the physical parameters.

```
wind advection dfdr -20.90 index 2
```

The **set dynamics** command (page 117 below) controls many details of the dynamics. The **set dynamics pressure mode** command tells the code whether it should search for globally subsonic or supersonic solution. If this is not specified the code will compare the ram and gas pressure at the illuminated face to try to determine whether a super- or sub-sonic solution is appropriate.

Convergence – the level of convergence can be estimated by comparing the discretization error and convergence error as function of iteration, as shown in Figure 4 of Henney et al. (2005).

12.3.3. wind 5 km/s no continuum

The **no continuum** keyword tells the code not to include continuous absorption in the calculation of the radiative acceleration.

12.4. Miscellaneous dynamics commands

12.4.1. set dynamics [options]

This changes some aspects of the dynamics solutions when advective winds are used.

set dynamics advection length [fraction] This sets the look-back distance used for the advection terms in the initial iterations of the solutions. Its optimum value is determined by a compromise between speed of convergence (which is improved for large lengths) and accuracy (which is improved for small lengths). The code automatically cuts the look-back distance when good convergence is obtained so a reasonably large value can be assumed initially.

If the keyword **fraction** occurs then the number on the line will be the fraction of the total depth of the model. It is the log of the fraction if it is negative. If **fraction** does not occur then the number is the log of the scale length in cm.

set dynamics antishock depth 16 would put an anti-shock at a depth of 10^{16} cm.

set dynamics antishock Mach 1.01 would put in an anti-shock when the mach number fell below 1.01.

set dynamics pressure mode This changes some aspects of how the pressure solver deals with the sonic point. The options are: **original**, **subsonic**, **supersonic**, and **strongd**. The default chooses subsonic or supersonic based on a comparison of the ram pressure and gas pressure at the face. **Original** mode uses similar criteria to choose in each zone but is liable to oscillation. **Subsonic** and **supersonic** will force a globally subsonic or supersonic solution. **Original** and **strongd** can pass through a sonic point. **Strongd** does this by following the supersonic branch until there is no valid pressure solution, then following the minimum of the pressure-density relation until it can leave along the subsonic branch. By varying the face conditions, the depth of the internal region of unphysical solution values can be minimized, to converge on a physical strong-D type solution.

set dynamics shock depth. The argument is the log of the shock depth in cm.

set dynamics relax 3. The argument is the first iteration to include dynamics or follow time-dependent behavior. The initial iterations are done to establish the equilibrium geometry, optical depth scale, and properties. The default is to do 2 iterations to relax the solution.

13. STOPPING CRITERIA

13.1. Overview

Cloudy will stop at some depth into the cloud. The physics that sets this depth is important since it can directly affect predicted quantities. This chapter describes various stopping criteria.

Two geometries, matter bounded and radiation bounded, can be identified for an ionized gas.

A radiation-bounded cloud is one where the outer edge of the emitting gas is a hydrogen ionization front. In this case the calculation stops because nearly all ionizing radiation has been attenuated and the temperature falls below 4000 K, the default lowest-allowed kinetic temperature. This choice of lowest temperature was made with optical emission lines in mind. Setting another outer limit is not necessary unless molecules or lines with very low ionization and excitation potentials (i.e., the [C II] or [O I] far infrared lines) are of interest. It would then be necessary to lower the stopping temperature with the **`stop temperature`** command (described on page 126 below).

In a matter-bounded cloud the gas is optically thin to energetic radiation and the outer radius of the cloud must be specified. This could be a column density, physical thickness in cm, or optical depth. More than one stopping criterion can be specified, and the calculation will stop when the first one is met.

Cloudy will say why it stopped after the results of the last zone calculation are printed. It is very important to make sure that the calculation stopped for the reason you intended.

If no stopping criteria are set the calculation will usually stop because the default lowest temperature (4000 K) or the default greatest number of zones (1400) was reached.

13.2. Danger! Understand why the calculation stopped!

Sometimes the predicted emission-line spectrum will depend strongly on the thickness of the cloud. The cloud thickness is set by the stopping criteria. The predicted intensity will depend on thickness if the outer edge of the cloud is within a line's creation region. This is often the case for some lines in an X-ray irradiated gas and for any radiation field and molecular or low-ionization infrared lines.

There are several checks that should be made to confirm that the spectrum is the one expected and not an artifact of the cloud thickness or stopping criteria. The first and most important is to understand *why* the calculation stopped. This is explained in the first comment after the last zone is printed. First locate the print out for the last zone. The following example, from the *pn_paris* simulation, shows the printout that includes the last zone’s results and the start of the calculation’s summary. The first line after the ionization distribution of iron gives the title for the model and the line after that gives the reason that the calculation stopped. In this case the calculation stopped because the kinetic temperature fell below the lowest temperature, which was left at its default of 4000 K. This occurs very near the hydrogen H^+ - H^0 ionization front. Optical and UV lines form at higher temperatures so the calculation would include all contributors to the optical/UV spectrum. Lines such as [C II] 158μ or [Si II] 34.8μ form in cool neutral gas, so these lines would become stronger if the calculation went more deepl, into cold neutral gas.

```
####150  Te:3.978E+03 Hden:3.000E+03 Ne:1.276E+02 R:4.062E+17 R-R0:3.062E+17 dR:5.658E+13 NTR:  5 Htot:4.094E-19 T912: 9.97e+07###
 Hydrogen      9.70e-01 2.97e-02 H+o/Hden 1.00e+00 3.57e-09 H-    H2 1.57e-07 5.07e-10 H2+ HeH+ 8.59e-08 Ho+ ColD 3.27e+19 8.86e+20
 Helium        8.77e-01 1.23e-01 1.81e-04 He I2SP3 4.78e-08 5.43e-16 Comp H,C 1.39e-26 3.59e-27 Fill Fac 1.00e+00 Gam1/tot 6.57e-01
 Carbon        2.50e-04 9.97e-01 3.12e-03 0.00e+00 0.00e+00 0.00e+00 0.00e+00 H2O+/O   0.00e+00 OH+/Otot 0.00e+00 Hex(tot) 0.00e+00
 Sulphur    0  7.02e-05 9.64e-01 3.56e-02 2.36e-06 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00
 Argon      0  7.82e-01 1.96e-01 2.24e-02 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00
 Iron       0  9.25e-06 9.97e-01 2.80e-03 3.42e-06 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00
    parispn.in Meudon Planetary nebula
   Calculation stopped because lowest Te reached.    Iteration  1 of  1
   The geometry is spherical.
  !Some input lines contained [ or ], these were changed to spaces.
  !Non-collisional excitation of [OIII] 4363 reached   2.35% of the total.
  !AGE: Cloud age was not set.  Longest timescale was 3.68e+012 s = 1.17e+005 years.
   Suprathermal collisional ionization of H reached 9.48% of the local H ionization rate.
   Charge transfer ionization of H reached 8.94% of the local H ionization rate.
```

Left on its own, the code will probably stop when the temperature falls below the default lowest temperature of 4000 K. This is what happened in the preceding example. This temperature was chosen for two reasons; a) collisionally excited optical and ultraviolet lines generally form in gas hotter than this (but infrared lines will form at far lower temperatures) and b) more than one thermal solution is possible for temperatures around 3000 K (Williams 1967), so thermal instabilities may result if the gas extends to cooler temperatures.

It is a good idea to check whether the predictions would change if the model were made thicker or thinner. It is safe to assume that a line's intensity does not depend on the thickness of the cloud if the final temperature is well below the excitation potential of the line or the gas is more neutral than the species of interest.

The chapter "Output" in Part 3 of this document lists all possible reasons for stopping.

13.3. radius inner =18 [thickness =16; parsecs; linear]

The **radius** command is discussed on page 79 above. The optional second number sets the thickness or outer radius of the cloud.

13.4. stop AV 12.1 [point, extended]

This stops a calculation at a specified visual extinction A_V. The value is the extinction in magnitudes at the isophotal wavelength of the *V* filter (5500Å). The number is the linear extinction in magnitudes unless it is negative, when it is interpreted as the log of the extinction. Note that there must be spaces before and after the key "**AV**".

Properties of grains are determined by the **grains** command (see page 58 above). The distinction between the extinction for a point versus an extended source is described on page 63 above and in section 7.6 of AGN3. By default the A_V specified with this command will be for a point source, which is the quantity measured in extinction studies of stars. The extended-source extinction, appropriate for extinction across a cloud, is specified with the keyword **extended**.

13.5. stop column density = 23 [neutral; ionized; total; ...]

This stops the calculation at the specified hydrogen column density *N*(H) [cm^{-2}]. There are several optional keywords which determine whether the column density is the total (the default), the ionized hydrogen column density, the neutral hydrogen column density, or several other column densities. The default stopping column density is 10^{30} cm^{-2}.

By default the number on the line is interpreted as the log of the column density. The keyword **`linear`** forces that interpretation.

13.5.1. stop column density 23

The number is the log of the total hydrogen column density (atomic, ionic, and all molecular forms), defined as the integral

$$N(\mathrm{H}) = \int \left\{ n\left(\mathrm{H}^0\right) + n\left(\mathrm{H}^+\right) + 2n\left(\mathrm{H}_2\right) + \sum_{other} n\left(\mathrm{H}_{other}\right) \right\} f(r)\, dr \ [\mathrm{cm}^{-2}] \tag{69}$$

where *f*(*r*) is the filling factor.

13.5.2. stop neutral column density 23

The number is the log of the atomic hydrogen column density

$$N\left(\mathrm{H}^0\right) = \int n\left(\mathrm{H}^0\right) f(r)\, dr \ \ [\mathrm{cm}^{-2}]. \tag{70}$$

13.5.3. stop ionized column density 23

The number is the log of the ionized hydrogen column density

$$N\left(\mathrm{H}^+\right) = \int n\left(\mathrm{H}^+\right) f(r)\, dr \ [\mathrm{cm}^{-2}]\ . \tag{71}$$

13.5.4. stop atom column density 21.3

In some PDR literature the atomic hydrogen column density is defined as the sum of H^0 and H_2. This command allows the calculation to stop as this summed column density, defined as

$$N\left(\mathrm{H}^0 + 2\mathrm{H}_2\right) = \int \left[n\left(\mathrm{H}^0\right) + 2n\left(\mathrm{H}_2\right) \right] f(r)\, dr \ [\mathrm{cm}^{-2}]\ . \tag{72}$$

This command was added by Nick Abel. Note that this counts each H_2 as two hydrogen atoms.

13.5.5. stop H/TSpin column density 17.2

This calculation stops at the specified integral

$$N\left(\mathrm{H}^0\right) / T_{spin} = \int \frac{n\left(\mathrm{H}^0\right)}{T_{spin}} f(r)\, dr \ [\mathrm{K\ cm}^{-2}]\ . \tag{73}$$

Note that T_{spin} is computed self-consistently, including the effects of pumping by the background continuum (usually the CMB) and the local Lα radiation field.

13.5.6. stop H2 column density 19.2

The calculation stops at the specified molecular hydrogen column density

$$N(\mathrm{H_2}) = \int n(\mathrm{H_2}) f(r) dr \ [\mathrm{cm^{-2}}] \ . \qquad (74)$$

The 2 in H_2 must come before the log of the column density in the command. This is really the H_2 column density, not twice it.

13.5.7. stop CO column density 19.2

The calculation stops at the specified column density in CO

$$N(\mathrm{CO}) = \int n(\mathrm{CO}) f(r) dr \ [\mathrm{cm^{-2}}] \ . \qquad (75)$$

This command was added by Nick Abel.

13.5.8. stop effective column density 23

This is actually a form of the **`stop optical depth`** command (see page 124 below). Usually, low-energy cutoffs in X-ray spectra are parameterized by the equivalent column density of a cold neutral absorber with cosmic abundances. Actually what is measured is an optical depth at some energy, generally around 1.0 keV. If the gas is ionized then a much larger column density will be needed to produce the observed absorption. The difference can be more than an order of magnitude. This command stops the calculation when the incident continuum has been attenuated by the appropriate absorption at 1.0 keV. The calculation stops when the absorption optical depth at 1.0 keV (neglecting scattering opacities) reaches a value of

$$\tau_{abs}(1.0\,\mathrm{keV}) = N_{effec} 2.14 \times 10^{-22} \ [\mathrm{Napier}] \qquad (76)$$

at 73.5 Ryd. The argument of this command is the log of the effective column density N_{effec}. The absorption cross-section per proton for cold neutral gas is taken from Morrison & McCammon (1983). Scattering opacities *are not* included in this optical depth. No attempt is made to use realistic physical conditions or absorption cross sections – this command follows the Morrison & McCammon paper.

If the gas is highly ionized then the actual column density will be greater than the effective column density. It will be less if the abundances of the heavy elements are greatly enhanced.

13.6. stop depth . ….

This is another name for the **`stop thickness`** command, described on page 126 below.

13.7. stop eden 3 [linear]

The calculation stops when the electron density falls below the indicated value. The number is the log of the electron density [$\mathrm{cm^{-3}}$]. The optional keyword **`linear`** will force the argument to be interpreted as the quantity itself, not its log. This command is one way to stop constant-temperature models. For instance, the calculation can be forced to stop at the H^+-H^0 ionization front by setting the stopping electron density to approximately half of the hydrogen density.

The following examples show a case that will stop near the He^{2+}-He^+ ionization front and a case that will stop near the H^+-H^0 ionization front for solar abundances.

```
//
// stop at the He++ - He+ ionization front
hden 9
stop eden 9.06 // stop when helium (10% by number) is He+

//
// stop at H+ - H0 ionization front
hden 5
stop eden 4.5 // stop when electron dens falls below H density
```

The default is an electron density of -10^{30} cm^{-3}. (The negative sign is not a typo.)

13.8. stop efrac = 1.05

The model will stop when the electron fraction, defined as the ratio of electron to total hydrogen densities, falls below the indicated value. This is another way to stop calculations at ionization fronts. This is useful if the hydrogen density there is not known beforehand as occurs in constant-pressure calculations. The argument is the fraction itself if it is greater than zero and the log of the fraction if it is ≤ 0.

The default is an electron fraction of -10^{37} cm^{-3}. (The negative sign is not a typo.)

13.9. stop line "C 2" 157.6m reaches 0.2 rel to "O 3" 5007

The calculation will stop when the emission line with the label given within the first pair of quotes and the wavelength given by the first number exceeds an intensity given by the second number, relative to an optional second emission line. In this example the calculation will stop when the intensity of [C II] 158 μm reaches 0.2 relative to [O III] λ5007. If a second optional line is not entered it will be *Hβ*[30]. This can be a useful way to stop matter-bounded models. The results of this command are not exact; the final intensity ratio will be slightly larger than the ratio specified.

The line label and wavelength should be entered exactly as it appears in the emission line output. The line label within the quotes must have the same number of spaces as in the output. "C 2" and "C 2" are not the same (the first has only one space and the second is correct with two spaces). The wavelength is assumed to be in Angstroms if no letter follows it. The wavelength can be changed to microns or centimeters by immediately following the wavelength with 'm' or 'c' as in 157.6m.

[30] The scaling of the line intensities can be changed with the **normalize** command, as described on page 128. That command can change both the normalization line (usually H*β*) and its relative intensity (usually 1). If the second line is not set with the **stop line** command then H*β* is the denominator in the ratio. The **stop line** command always uses the ratio of the two line intensities on the scale that is set with the **normalize** command. In versions C07.02 and before the **normalize** command did not interact with the stop line command.

Up to 10 different **`stop line commands`** may be entered. If more than one **`stop line command`** is entered then the code will stop when any limit is reached.

13.10. stop mass 32.98

The calculation will stop when the total mass of the computed structure exceeds the quantity entered. If the inner radius is specified (the luminosity case) then the entered number is the log of the mass in gm. If the inner radius is not specified (the intensity case) then it is the log of the mass per unit area, gm cm^{-2}.

At the current time no attempt is made to make the computed mass exactly equal to the entered number. The calculation will stop after the zone where the mass is first exceeded.

13.11. stop mfrac = 0.5

The calculation stops when the hydrogen molecular fraction, defined as $2n(H_2)/n(H_{tot})$, exceeds the indicated value. This is a way to stop calculations within a PDR. The argument is interpreted as the molecular fraction itself if it is greater than zero and as the log of the fraction if it is less than or equal to zero.

The default is a molecular fraction of 10^{37} cm^{-3}.

13.12. stop molecule depletion -2

Nick Abel incorporated the condensation of molecules onto grain surfaces. Currently CO, H_2O, and OH condensation are treated. The density of molecules on grains is given as a species with the molecule's usual label, “CO”, “H2O”, or “OH”, followed by the string “gr”. The rates of UV and cosmic ray desorption along with accretion come from Hasegawa, Herbst, & Leung (1992) and Hasegawa & Herbst (1993). The grain surface chemistry mentioned in these papers is not included so our treatment of condensation is closer to the work of Bergin, Langer, & Goldsmith (1995), who also use the Hasegawa et al. rates. Use the **`no grain molecules`** command (page 202 below) to turn off this condensation.

13.13. stop nTotalIoniz 100

This is a way to stop a calculation while debugging and is not normally used. The variable with this name is incremented each time the ionization evaluation routine is called. This command will cause the calculation to abort after the specified number of calls.

13.14. stop optical depth -1 at 2.3 Ryd

This command stops the calculation at an arbitrary continuum *absorption* optical depth. The first number is the log of the optical depth. The optical depth is interpreted as a log by default. If the **`linear`** keyword occurs then the number is interpreted as the linear value. The optical depth is only for absorption and does not include scattering opacities. The second number is the energy in Rydbergs. It is interpreted as a log if it is negative, as linear if positive, and must be within the energy bounds considered by the code (presently 1.001×10^{-8} Ryd to 7.354×10^{6} Ryd).

At present only one stopping optical depth can be specified. If more than one is entered then only the last is honored.

It is traditional in X-ray astronomy to characterize low-energy cut-offs as the equivalent *completely neutral* column density for *solar* abundances. This is not correct when the gas is ionized (since the high-energy absorption opacity is diminished) or when the abundances of the heavy elements are enhanced (since the high-energy opacity is increased). For extreme cases these effects can change the opacity by more than an order of magnitude. The deduced column density is underestimated by the same amount. It is better to convert the deduced column density back into an optical depth at 0.5 or 1 keV (this is actually the observed quantity) and use this optical depth and energy as the stopping criteria than to use the deduced column density as a stopping criterion. Either this command, or the **`stop effective column density`** command (which is actually a form of the **`stop optical depth`** command, see page 121 above) can be used to stop the calculation at an X-ray optical depth corresponding to a certain low-energy absorption.

The optical depth used in this command is the absorption optical depth and does not include scattering opacities. In general, the effects of scattering opacities are much more geometry dependent than absorption opacities.

13.14.1. stop Balmer optical depth = -.3

This command is a special case of the **`stop optical depth`** command in which the energy does not need to be specified but the keyword **`Balmer`** is given. It will stop the calculation when the log of the absorption optical depth at the Balmer continuum threshold (ν = 0.250 Ryd) reaches the specified value. The default is $\tau_{Bac} = 10^{20}$ and the optical depth is always interpreted as a log. This is the *total absorption* optical depth at the Balmer edge and includes all computed absorption opacity sources such as grains or free-free absorption, but neglects scattering.

13.14.2. stop Lyman optical depth = 5

This is a special case of the **`stop optical depth`** command in which the energy does not need to be specified but the keyword **`Lyman`** is given. The number is the log of the Lyman limit optical depth, τ_{912}. The default value is $\tau_{912} = 10^{20}$. The stopping criterion is *really* the *total* 912Å *absorption* optical depth and *not* the hydrogen Lyman limit optical depth at 912Å. These are not exactly the same, especially when grains are present or the abundances of the heavy elements are enhanced.

13.14.3. stop 21cm optical depth = linear 3

This stops the calculation when the *line center* optical depth of H I λ21 cm reaches the entered value. The populations of the hyperfine levels are determined by solving the full level populations with the effects of pumping by Lα and the external continuum included. The calculation stops when the optical depth from the continuum source to the outer edge of the cloud exceeds the entered value. The actual optical depth with be greater than or equal to the indicated value.

Note that Cloudy always uses the dimensionless *line center* optical depth. The *integrated* optical depth is the standard used in radio astronomy. The *integrated* optical depth is called the *mean* optical depth in optical spectroscopy. The dimensionless mean optical depth is $\sqrt{\pi}$ larger than the line center optical depth. In radio astronomy, the integrated optical depth is often given in velocity units, km s^{-1}.

13.15. stop pfrac = 0.23

The calculation will stop when the proton fraction, defined as the ratio of proton (ionized hydrogen) to total hydrogen densities, falls below the indicated value. This is another way to stop calculations at ionization fronts and is useful if the hydrogen density there is not known beforehand. This occurs in constant pressure calculations, for instance. The argument is interpreted as the fraction itself if it is greater than zero and the log of the fraction if it is less than or equal to zero.

The default is an proton fraction of -10^{37} cm^{-3}. (The negative sign is not a typo.)

13.16. stop temperature 1,000K [linear, exceeds]

The calculation will stop when the kinetic temperature drops below T_{low}, the argument of this command. The argument is interpreted as the log of the temperature if ≤ 10 and as the linear temperature if > 10 or if the **linear** keyword appears.

The default value is T_{low} = 4000 K. Gas cooler than this produces little optical emission, but may be a strong emitter of infrared lines such as the [C II] 158 μm or the [O I] ^3P lines. The lowest temperature allowed, T_{low}, should be adjusted with this command so that the excitation potential $h\nu$ is $\cong kT_{low}$ for the lowest excitation potential transition considered. Note that more than one temperature is sometimes possible when $T \approx 10^3$ K (Williams 1967) so thermal stability problems may develop if T_{low} is lowered below a few thousand degrees Kelvin. This issue is discussed further in a section in Part 3 of this document.

If the keyword **exceeds** appears on the line then the specified temperature will be the highest allowed temperature. The calculation stops if the temperature *exceeds* the value on the command. This might be necessary when a grid of models is computed but those in the high temperature phase (i.e., $T > 10^5$ K) are not of interest. The other rules for the command are unchanged.

If no number appears on the command line, but the keyword **_off** does, then temperature will not be used as a stopping criterion.

13.17. stop thickness 9.3 [parsecs; linear; 23 on sec iter]

This sets an upper limit to the thickness of the cloud. The argument is interpreted as the log of the thickness unless the keyword **linear** appears. The default units are centimeters but it will be interpreted as the log of the thickness in parsecs if the keyword **parsec** appears on the line.

The **stop thickness** command has the same effect as the optional second number on the **radius** command (page 79 above). This command makes it possible to set a cloud thickness when the inner radius is not specified, such as when the ionization parameter is given.

Any number of thicknesses may be entered on the command line. Each will be the ending thickness for consecutive iterations. The limit to the number of stopping values is set by the limit to the number of iterations that can be performed. If fewer numbers are entered than iterations performed then the last number will be used for all further iterations.

The keyword **`depth`** can be used instead of **`thickness`**.

13.18. stop velocity < 1 km/s

The calculation will stop if the absolute value of the wind velocity falls below the value. The stopping velocity is entered in km s^{-1} but is converted to cm s^{-1} within the code.

13.19. stop zone 123 [21 on sec iteration, ...]

This sets a limit to the number of zones that are computed on each iteration. It is not normally used. In this example the calculation will stop after computing 123 zones. The default value is 1400. Any number of zones may be entered, each being the ending zone for consecutive iterations. This limit is set by the limit to the number of iterations that can be performed. If fewer numbers are entered than iterations performed then the last number will be used for all further iterations.

The code checks that it did not stop because the default number of zones was reached. A warning will be generated if this happens since it was probably not intended. Use the **`set nend`** command (see page 214 below) to increase the default number of zones while keeping this checking active.

The code allocates memory to store a great deal of information for the limiting number of zones. Increasing the number of zones will also increase the memory needed to run the code. Don't do this unless you really need to use the zones.

14. CONTROLLING OUTPUT

14.1. Overview

Cloudy is capable of generating lots of output although its default output is minimal. Commands that control the output are described here. The section "Output" in Part 3 of this document describes the meaning of the output.

14.2. no buffering

Output will be lost if the code crashes before ending because of the way that the C++ language handles file buffering. There is a **`no buffering`** command, described on page 128 above, which forces output to be saved to disk as soon as it is created. This slows down the execution time considerably but may need to be used to save results when diagnosing a crash. If this command is used on most systems output will no go to *stdout* but will go to *stderr* instead. *stderr* can be directed to a file by redirection of 2 as in the following example

```
cloudy.exe < sim.in > sim.out 2>sim.err
```

14.3. normalize to "O 3" 5007 [scale factor = 100]

The strength of an emission line in the standard output will be given in intensity or luminosity units and as its intensity relative to a reference line. In the main printout each emission line has a label and wavelength, followed by the energy radiated in the line, ending with the intensity relative to a reference line.

Emission-line intensities are usually listed relative to the intensity of Hβ λ4861Å, the default reference line. By default the reference line has an intensity of unity. This command can change the reference line to any of the other predicted lines and can change the relative intensity of the reference line to another value. The relative intensities of all lines in the spectrum will be relative to the intensity of the line whose label is within the double quotes and with wavelength given by the first number. The label must be the four-character string that identifies the line in the print out[31] and the wavelength must match the printed wavelength to all four figures. The wavelength units must appear if they are not Angstroms.

The optional second number sets the relative intensity of the reference line. If it is equal to 100, as in this example, then all intensities will be relative to a reference line intensity of 100. The default is for an intensity of unity. The example given above will cause the relative intensities to be expressed relative to an [O III] λ5007 intensity of 100. The scale factor must be greater than zero.

The code works by finding the first line in the emission-line stack whose wavelength and label matches the line on this command. There is a possible uniqueness problem since more than one line can have the same wavelength. This is especially true for XUV or soft X-ray lines and for H_2 lines.

[31] The label was optional in versions 94 and before of the code, but now is required due to the large number of lines, making unique wavelengths unusual.

The following shows some examples of the **normalize** command:

```
// normalize to spectrum to Pa
normalize to 1.875m

// normalize spectrum to the [OI] IR line on a scale where it is equal to 100
normalize to “O  1” 63.17m = 100
```

14.4. plot [type, range]

Plots of several predicted quantities can be made. One of the keywords described below must appear on the command line. Up to 10 plots can be generated. The keyword **trace** will turn on a great deal of information concerning the mechanics of generating the plot.

Publication-quality plots can be produced using the **punch** commands (described beginning on page 138 below) to produce a file that can then be post-processed using other plotting software.

14.5. plot continuum [_raw, trace, range][32]

This plots the continuum. This energy range can be changed by entering the **range** key and the lower and upper limits. This is described in detail in section 14.6.1 below.

The default is to plot both the incident continuum (in units of νf_ν) (plotted as .'s) and the transmitted continuum (the o's). If the option **raw** is specified then the continuum in units actually used inside Cloudy (cm^{-2} s^{-1} cell^{-1}) will be plotted. If the keyword **photon** appears then the units of the plotted continuum will be photons cm^{-2} s^{-1} Ryd^{-1}.

14.5.1. plot continuum keywords

It is possible to plot specific components of the continuum with the following series of keywords.

14.5.2. plot diffuse continuum

This plots the diffuse emission per unit volume within the last computed zone. This gives emission by gas and grains in the optically thin limit and unity filling factor.

14.5.3. plot emitted continuum

The net integrated continuum produced by the cloud is plotted. This is the sum of the continua emitted in the inward and outward directions from the computed ionization structure and does not include the incident continuum.

[32] Today most plots are generated by producing punch output then post-processing that output in other software. The plot commands described here still function but are likely to be removed in a future version of the code.

14.5.4. plot outward continuum

The contents of the ***outcon*** and ***flux*** arrays, multiplied by the local gas opacity, are plotted to indicate sources of ionization and heating.

14.5.5. plot reflected continuum

The continuum emitted from the illuminated face of the cloud is plotted. This includes the back-scattered portion of the incident continuum along with the diffuse continuum emitted from the cloud in the direction towards the central object. This is possible only for non-spherical (open) geometries.

14.6. plot opacity [type, range]

The opacity (total cross section per hydrogen atom) of the first and last zones is plotted. The full continuum predicted by the code, the range 1.001×10^{-8} Ryd $\leq h\nu <$ 7.354×10^{6} Ryd, is plotted by default. This is changed by using the **range** option.

There are three optional keywords; **absorption**, **scattering**, and **total**, to change which opacity is plotted. If none appear then the total opacity is plotted.

14.6.1. plot range options

The keyword **range** specifies the energy range of the **opacity** and **continuum** plots. If one number occurs on the line then it is the lowest energy in Rydbergs. If the first number is zero then it is replace with the lowest energy in the continuum, 1.001×10^{-8} Ryd. The optional second number is the highest energy shown on the plot. If it is omitted or zero then the high-energy limit of the code, presently 7.354×10^{6} Ryd, is used. If either number is negative then both are interpreted as the logs of the energies, otherwise they are assumed to be the linear energy. If the first number is zero (i.e., interpreted as the lowest energy considered by the code) then the second number is interpreted as the energy of the upper limit to the plot and not its log.

The following give specific examples of the range option.

```
// plots the absorption opacity between 0.1 to 10 Ryd.
plot absorption opacity, range=.1 to 10 Ryd
//
// plot the opacity between 1 Ryd and
// the high energy limit of the code.
plot scattering opacity, range=1
//
// the range will be the full energy limit of the code
plot opacity
```

14.7. plot _map [Tmin=3,000K, Tmax=20,000K, linear, range]

The keyword **_map** (note the leading space) says to do a plot of the heating and cooling rates [erg cm^{-3} s^{-1}] as a function of temperature for the last computed zone. The **punch map** command (page 165 below) saves this information in a file and is more useful.

14.7.1. plot map range options

The high and low temperatures on the map are changed with the keyword **range** and one or two optional numbers. If no number appears then a temperature range of

10 K to 10^9 K is used. If only one number appears then only the lower temperature limit is changed. If two numbers appear then both lower and upper limits are changed.

If the first number is ≤ 10 then both numbers are interpreted as logs of the temperature. If the first number is > 10 then both are interpreted as the temperature itself. If the keyword **`linear`** appears then both numbers are interpreted as the temperature itself no matter how large or small they may be.

The number of points on the map is set with the **`set nmaps`** command described on page 215 below.

14.8. print ages

The code normally assumes that the system is old enough for microphysical processes to have become time steady. This tells the code to print all of the timescales tracked by the code. These are the same timescales considered by the **`age`** command (page 75 above). Normally only the shortest timescale is printed at the end of the calculation.

If a physical process is not significant, for instance, the H_2 formation timescale in a 10^6 K gas, the age is still computed but is set to a negative number. This retains the value while not including the process when the important timescales are determined.

14.9. print arrays

This tells the code to print the array elements that enter into solutions of the ionization balance. By default it will print this information for all elements. If the keyword **`only`** appears then it will also look for the name of an element and will only print the arrays for that element. This is a debugging aid.

14.10. print citation

Cloudy is a research project that involves the creative efforts of many people. It should be cited as follows: "Calculations were performed with version yy.mm.dd of Cloudy, last described by Ferland et al. (yyyy)." The numbers represent the release date and the citation is to a review paper. The citation should mention the version of the code since some predictions changes as the atomic data and treatment of physical processes improve. Old versions of the code are never deleted from the web site so it is possible to recover a version that produced a given result.

This command will print the current version number of the code and give the full bibliographic citation for the review paper.

14.11. print constants

The physical constants stored in the header file *physconst.h* will be printed along with sizes of some variables on your computer.

14.12. print column densities [on; off]

This controls whether the column densities of the various constituents are printed. The keywords are **_ON_** and **_OFF**. The default is to print the column densities.

The column densities of several excited states within ground terms of some species are printed as well. The meaning of the labels for the excited states column densities is given in the discussion of ***cdColm*** in Part 3 of this document.

14.13. print coolants, zone 135

This prints the coolants for the specified zone. If no zone number or 0 appears on the line then the coolants for *all* zones will be printed. The total cooling and the fractional contribution of the strongest coolants are printed. For each coolant a label gives an indication of the spectroscopic origin of the coolant and the following integer gives its wavelength, with a 0 to indicate a continuum. The last number of the group is the fraction of the total cooling carried by that agent.

14.14. print continuum [options]

This is actually two very different commands, with different purposes. The second form will eventually be removed.

14.14.1. print continuum

When no other options appear the **print continuum** command will print the sum of the total emitted and inward reflected continuum as a series of entries in the standard emission line array. Each has a label *nFnu*. This is the emission produced by the cloud and does not include the attenuated incident continuum. The entry *nInu* is the transmitted plus reflected portion of the continuum. The **set nFnu** command (page 214 below) provides a way to change which contributors are included in this prediction.

If the **print line inward** command (page 136 below) also occurs then the total inward emission (the label “InwT”) and the reflected incident continuum (label “InwC”) will also be printed.

The energies that are printed is stored in the vector ***EnrPredCont*** that is initialized with ***NPREDCONT*** points. These can be changed to obtain the continuum at other energies by editing the source.

14.14.2. print continuum block

If the keyword **block** appears then the code will print the transmitted continuum at the end of the calculation. The information includes the integrated Balmer and Lyman continua, the transmitted X-ray continuum, and frequency-by-frequency continuum intensities.

The **punch continuum** command (page 143 below) provides this information in a far more useful format. This option on the **print continuum** command will be removed in a future version of the code.

14.14.3. print continuum indices

The file created by the **punch continuum** command (page 143 below) identifies a line that occurs within each continuum bin. This can be used to understand what lines contribute to the predicted spectrum. The line label is for the first line that was entered in a particular cell. It is not the strongest line and there may be many lines contributing to a particular cell. This command will print the line energy (Rydberg), continuum array index, and the line's spectroscopic notation, for every line that is included in the calculation. The lines will be printed in the order in which they are entered into the continuum. The printout can then be sorted by energy or array index to discover all lines that occur within a particular cell. This is a debugging aid.

There are two optional numbers which give the lower and upper limit to the energy range (Rydbergs) to be printed. All lines are printed if these numbers do not appear then.

14.15. print departure coefficients

LTE departure coefficients for levels within an element along the H-like or He-like isoelectronic sequences will be printed. The **print populations** command (page 134 below) controls printing individual level populations.

If the keyword **He-like** appears then an element on the helium-like isoelectronic sequence will be printed. Otherwise an element of the H-like isoelectronic sequence is chosen. The code will search for the name of an element, and if it finds one, will print only that element. If no elements are recognized then departure coefficients for H^0 (the H-like sequence) or He^0 (the He-like) are printed.

14.16. print errors

The code will always identify problems by either printing comments during the calculation or warnings after the calculation is complete. This says to also print these warnings to ***stderr***. On many systems this output can be redirected to the screen. See the **no buffering** command on page 128 above to see how to handle stderr output.

14.17. print every 1000 [5 37 93]

Cloudy will always print the results for the first and last zones. This command varies the number of zones printed between these two. If more than one number is entered then each applies to successive iterations. The example above will print every 1000 zones on the first iteration, every 5 zones on the second iteration, 37 on the next, etc. If there are fewer numbers entered than iterations performed then the last number entered will be used for all further iterations.

14.18. print heating

The relative heating due to each stage of ionization or physical process is printed. This is the fraction of the total heating due to this particular stage of ionization and is printed directly below the relative abundance of that stage.

14.19. print populations [H-like carbon, to level 45]

Level populations are normally not printed for the atoms and ions of the H-like or He-like isoelectronic sequences. This will print them. If no numbers appear on the line then the first 15 levels will be printed. Enter the highest level to print on the line as an integer if more are desired.

If the keyword **`He-like`** appears then an element on the helium-like isoelectronic sequence will be printed. Otherwise an element of the H-like isoelectronic sequence is chosen. The code will search for the name of an element, and if it finds one, will print that element and isoelectronic sequence. If none are recognized then populations for H I are printed.

The departure coefficients are printed with the **`print departure coefficients`** command (page 133 above).

14.20. print last

Normally results for every iteration are printed as they are computed. This command says to print only results for the last iteration.

14.21. print line *options*[33]

A large block of emission-line intensities is printed after the calculation is complete. This controls details of that printout.

Some options change the layout of this information. These include options to print a single column, to sort the lines by wavelength or intensity, or to print only the strongest lines, or those within a certain wavelength range.

Other options indicate line formation processes. A great deal of information about line formation and beaming is stored within the code but not normally printed to save space. The section of Part 3 of this document *The Emission Lines* gives more information.

Some spectra have so many lines that several different transitions may appear to have the same wavelength. This occurs to some extent for most H_2, Fe II, and He-like spectra. The **`set line precision`** command, described on Page 213 below, allows you to change the number of digits in the printed line wavelength. It may be necessary to increase the wavelength precision if the default line wavelengths are ambiguous and more than one transition appears with the same wavelength.

14.21.1. print line all

All of the contributions to line formation, including collisions, pumping, and heating, will be printed.

[33] In versions 87 and before, the code printed some relative line intensities for each zone. An extra line could be added with the **`print line`** command. This command, and that printout, no longer exists. Use the **`punch line intensities`** command instead.

14.21.2. *print line cell xx*

More than one line can occur within a continuum cell in the output produced by the **punch continuum** command (see page 143 below). This command will print the label for every line that falls into a particular continuum cell. The number of the cell, with the lowest energy cell being 1, must appear.

14.21.3. *print line collisions*

Collisions are often the dominant contributor to an optically thick resonance line. This adds an entry with the label "Coll" followed by the wavelength and the collisional contribution.

14.21.4. *print line column [linear]*

The main block of emission lines is normally printed with four lines across the page. This command says to print lines as a single column to make it easier to enter into a spreadsheet. The keyword **linear** will cause the intensities to be printed as the linear flux in exponential format rather than as the log.

14.21.5. *print line emergent*

The code distinguishes between intrinsic and emergent line intensities. By default the intrinsic intensity is given for most output options. If this command appears then the emergent intensity will be given instead.

14.21.6. *print line faint -2 [_off]*

Cloudy will normally print the intensities of all emission lines with intensities greater than 10^{-3} of the reference line, which is usually Hβ. This changes the limit to the relative intensity of the weakest line to be printed. The argument is either the log (if ≤ 0) or the linear (if positive) intensity of the weakest line to print, relative to the reference line. The reference line is usually Hβ, and can be changed with the **normalize** command (page 128 above). In the case shown here, only lines with intensities greater than 1% of Hβ will be printed.

If no numbers are entered, but the keyword **_off** appears then all lines are printed, even those with zero intensity.

14.21.7. *print line flux at Earth*

If the distance to an object is set with the **distance** command (page 78 above), and line luminosities are predicted (see the discussion on page 10 above) then this command says to print the observed flux at the Earth rather than the line luminosity. The units are ergs cm^{-2} s^{-1}. (No interstellar extinction is included, of course). Both the keywords **flux** and **Earth** must appear. This command can be combined with the **aperture** command (see page 75 above) to simulate observing only part of a spatially-resolved object.

14.21.8. *print line heat*

Fluorescent excitation is included as a line formation process. If a line is radiatively excited but then collisionally deexcited it will heat rather than cool the gas. This option prints the heating due to line collisional de-excitation. The entry will have the label "Heat" followed by the wavelength.

14.21.9. print line H2 electronic

By default only ro-vibrational lines within the ground electronic state of H_2 are included in the emission-line printout when the large H_2 molecule is included with the **`atom H2`** command (page 85 above). This command tells the code to also print electronic transitions.

14.21.10. print line inward

Optically-thick emission lines are not emitted isotropically. The "inward" fraction of the line is the part that is emitted from the illuminated face of the cloud into the direction towards the source of ionizing radiation. This will generally be greater than 50% of the total intensity if the line is optically thick. This command prints this inward fraction with the label "Inwd" followed by the wavelength.

14.21.11. print line optical depths [_off, faint]

Line optical depths are not printed by default. The option tells the code to print them at the end of the iteration. There are two optional keywords.

If **`_off`** appears then line optical depths will not be printed. This is useful if turned on in a previous iteration and no longer needed.

The keyword **`faint`** sets the smallest line optical depth to print. The default smallest line optical depth to print is 0.1. The log of the limit must be given. Optical depths for all lines that mase are printed.

14.21.12. print line pump

All lines include fluorescent excitation by the attenuated incident continuum as a line formation process. Continuum pumping will often be the dominant formation mechanism for optically-thin high-excitation lines. This option prints an estimate of the contribution to the total line intensity from this process. The entry will have the label "Pump" followed by the wavelength.

14.21.13. print line sort wavelength [range 3500A to 1.2m]

The output spectrum to be sorted by wavelength rather than by ion[34]. It was originally added by Peter G. Martin. If the **`range`** option appears then two more numbers, the lower and upper bounds to the wavelength range, must also appear. Each number is interpreted as the wavelength in Angstroms by default, but is interpreted as the wavelength in microns or centimeters if the wavelength is immediately followed by a "c" or "m". The two wavelengths must be positive and in increasing wavelength order.

[34] The **`print sort`** command existed but did not function between 1986 and 2001. It became functional again with version 96 but was moved to become an option on the **`print line`** command..

14.21.14. print line sort intensity

The predicted emission lines will be sorted in order of decreasing intensity.

14.21.15. print line sum

This prints the sum of the intensities of an arbitrary set of emission lines. This can be useful for applications such as the Stoy (1933) energy balance method of determining stellar temperatures, which rely on the sum of a set of observed line intensities relative to a recombination line (see also Kaler & Jacoby 1991 and section 5.10 of AGN3). The sum is printed as the last entry in the emission-line array as an entry with the label “Stoy” and a wavelength of 0.

Each emission line included in the sum is entered on its own line. This list begins on the line after the **`print line sum`** command and continues until a line with **`end`** in the first three columns appears. The line label must occur as the first four characters on each line and the line wavelength must appear as it does in the printout. The default units of the wavelengths are Angstroms and any other units must be specified. The following gives an example of its use.

```
print line sum
o  3 5007
totl 3727
o  1 6300
O  3  51.80m
S  3  18.67m
s  3 9532
end of lines
```

Up to 30 lines can be entered into the sum.

14.21.16. print line surface brightness [arcsec]

By default the line intensities that are printed after the calculation is complete is given as *L* with units erg s^{-1} for the luminosity case or $4\pi J$ [erg cm^{-2} s^{-1}] in the intensity case. This command will change these intensities into surface brightness units. The default is per steradian but if the keyword **`arcsec`** appears then the surface brightness will be per square arcsec.

14.22. print off

This turns off the print out, as with the **`print quiet`** command (page 138 below). This is normally paired with a later **`print on`** command to avoid printing parts of the output.

There is a possible problem. The code can read its own output as input, to make it easy to rerun a model. In many initialization files the following pair of commands appears:

```
print off
commands ….
print on
```

The resulting output will print the first **`print off`** command, but will not print the commands or the **`print on`** command. If this output is used as input no further output will be created for the new model. This problem will not occur if the **`print off`** command includes the keyword **`hide`**, described on page 16 above.

14.23. print on

This command turns on printout. This is the opposite of the **`print quiet`** or **`print off`** commands.

14.24. print only [header, zones]

The keyword **`only`** shortens the printout somewhat by stopping the calculation prematurely. If it appears then another keyword, **`header`** or **`zones`**, must also appear. The command **`print only header`** will cause the code to stop after printing the header information. The command **`print only zones`** will cause the code to return after printing the zone results on the first iteration. In both cases the calculation ends during the first iteration.

14.25. print path

The path giving the location of the data files will be printed.

14.26. print quiet

This sets Cloudy's quiet mode, in which nothing is printed at all. Printing can be turned off and then restarted at a particular zone by using the **`print starting at`** command described below.

14.27. print short

This shortens the detailed final printout. Only the emission lines and a short summary of some thermal properties of the model will be printed.

14.28. print starting at 61

This option turns off *all* printout *until* the specified zone is reached. This should come last in the input stream since command lines appearing after it will not be printed.

14.29. print version

This prints the code, compiler, and operating system versions, along with other information.

14.30. punch commands

14.30.1. Overview

Punch commands save results into a file that can be used later. They are the primary output mechanism for Cloudy. There are many options. For instance, physical quantities as a function of depth into the cloud, including temperature, ionization, and density, can be saved for later plotting. The continuum or other quantities predicted by the code can be output. The general idea is for the file produced by this command to then be post-processed by other plotting or analysis programs to produce final results.

One keyword must appear and only one keyword per line is recognized. Up to 100 **punch** commands can be entered.

14.30.2. An output file name must appear inside double quotes

Each **punch** command must specify a file name[35] for the resulting output. This file name must appear between a pair of double quotes as in "output.txt". It must be a valid file name for your operating system. The following is an example.

```
punch overview "model.ovr"
```

The code will stop if a valid file name is not present.

A prefix can be set for all filenames with the **set punch prefix** command, described on 216 below.

14.30.3. The "last iteration" option

Each **punch** command also has a keyword **last** that will cause the output to only be produced on the last iteration. It this keyword does not appear then output will be produced for every iteration. The results of each iteration are separated by a line of hash marks ("###").

14.30.4. The "no buffering" option

If the option **no buffering** appears then file buffering will be turned off for that file. This slows down the output considerably but ensures that all output will exist if the code crashes. There is also a stand-alone **no buffering** command (see page 128 above) to turn off buffering for the code's standard output.

14.30.5. The "clobber/no clobber" option

When the code is used as a stand-alone program to compute a single model it will open the punch file at the start of the calculation and close it at the end. In a sequence of models as in an optimization run this will happen for each new model and so will overwrite results of all previous calculations.

The **no_clobber** keyword on the **punch** command will produce one long file containing results of consecutive models. It tells the code to never close the file at the end of any but the last calculation and not try to reopen this file once it is open.

The default, with one exception, is to overwrite files. The **grid** command (see page 154 below) computes a series of simulations with a single input file. The entire set of output is usually needed so the default in this single case is to not overwrite files, but rather produce one large file.

Include the **clobber** keyword if you want to overwrite files, and the **no clobber** keyword if you want one large punch file with successive predictions.

[35] In versions 90 and before Fortran default punch units, with names like fort.9, could be used for punch output. The filename must be specified with versions 91 and later.

14.30.6. The "no hash" option

When more than one iteration is done the results of each iteration end with a series of hash marks, "`###`", to make the start of each iteration easy to find in an editor. These hash marks can cause problems if the file is then read in by other programs. The hash marks will not be produced if the **`no hash`** keyword appears.

The character string that is printed between iterations can be changed with the **`set punch hash`** command described on 216 below.

14.30.7. The "title" option[36]

The title of the model and the version number of the code will be printed on the first line of the punch file.

14.30.8. Depth versus radius

The code and this documentation make a consistent distinction between depth and radius. This is described on page 8 above. The *radius* is the distance from a point in the cloud to the center of symmetry, generally the center of the central object. The *depth* is the distance from a point in the cloud to the illuminated face of the cloud. In both cases the distance is to the center of the current zone.

The output from each punch command is described in the following sections. In those cases where quantities are given as a function of position into the cloud, the first column will usually give the depth, not the radius. You need to add the inner radius of the cloud to the depth to get the radius.

14.31. punch abundances

The log of the gas-phase densities [cm^{-3}] of the elements will be punched for each zone. This is the sum of the abundances of a chemical element in atoms, ions, molecules, and ices, but does not include grains. This provides a check for the effects of the **`element table`** (see page 57 above) and **`fluctuations abundances`** (see page 57 above) commands.

14.32. punch ages

The timescales for several physical processes will be punched as a function of depth.

14.33. punch agn [options]

This produces output files that were used to create data tables in the 2rd edition of *Astrophysics of Gaseous Nebulae*, referred to as AGN3 here. The options are the following: **`charge`** transfer, **`recombination`** coefficients, **`recc`** for hydrogen recombination cooling, **`opacity`**, **`hemis`**, and **`hecs`** (for He^0 collision strengths).

[36] The title was printed by default in versions 95 and before of the code. The title was generally deleted so that the punch file could be used to make plots so it is now missing by default.

14.34. punch asserts

The **assert** command is described on page 187 below and provides an automated way to validate the predictions of the code. Normally the results from these checks will be printed on the standard output. If this command appears then the same output will also be sent to a file.

14.35. punch average …

This reports averages of various quantities. It was included as a way to bring together information generated with the **grid** command (discussed on page 154 below).

The **punch** command is followed by a series of lines which say which average to generate. These end with a line that starts with the word **end**. The following is an example:

```
punch averages, file=”hii.avr” last no clobber
temperature, hydrogen 1 over volume
ionization, helium 2 over radius
column density oxygen 3
end of averages
```

14.35.1. Temperature average

The keyword **temperature** begins the line. The average temperature can be weighted with respect to any atom or ion. The name of one of the elements and the ionization stage, 1 for the atom, 2 for the first ion, etc, then follow.

The code computes averages weighted over radius or over volume. If the keyword **volume** appears then the volume-weighted mean temperature will be reported. The default is weighting over radius. The log of the temperature is reported.

The command works by calling ***cdTemp*** described in Part 3 of this document. It has all the options described there.

14.35.2. Ionization average

This reports the average ionization fraction of an atom or ion. The keyword **ionization** begins the line. It is followed by the name of one of the elements, then the ionization stage, 1 for the atom, 2 for the first ion, etc.

The code computes ionization fractions weighted over radius or over volume. If the keyword **volume** appears then the volume-weighted fraction will be reported. The default is weighting over radius. The log of the ionization fraction is reported.

The hydrogen molecular fraction $2n\left(\mathrm{H}_2\right)/n\left(\mathrm{H}_{tot}\right)$ can be obtained by asking for ionization stage 0 of the element hydrogen. This is a special case. Other molecular fractions cannot now be obtained.

14.35.3. Column density

The log of the column density of any atom or ion is reported. The keyword **column density** begins the line. It is followed by the name of one of the elements, then the ionization stage, 1 for the atom, 2 for the first ion, etc.

14.36. punch chemistry options

14.36.1. punch chemistry rates [molecule]

This command punches rates for various molecules. Following are recognized. These were implemented by Nick Abel.

punch chemistry rates CO The rates for various reactions involving CO are produced.

punch chemistry rates OH The rates for various reactions involving OH are produced.

14.37. punch column density

The logs of the column densities [cm^{-2}] of the gas constituents are punched.

punch column density will cause the large table of column densities that is printed in the main output at the end of the calculation to also be produced in a punch file.

punch some column densities allows you to specify which column densities to output. The code reads in a series of lines that give chemical elements and ionization stages. These end with a line that starts with **end**. The logs of the column densities of these species will be output in one line with each column density separated by a tab character. The following is an example:

```
punch some column densities “test.col”
hydrogen 2
helium 2
carbon 2
end of column densities
```

The name of a chemical element must appear in the first four columns of each line and be followed by the ionization stage. One is the atom, 2 the first ion, etc.

The column densities in molecules or in levels within an ion can be obtained. The command works by saving the first four letters on each line together with the ionization stage. These are then passed as the first two arguments to ***cdColm***, a routine described in the Chapter *Cloudy as a Subroutine* in Part 3 of this document. That section describes how to find molecular or state-specific column densities. If the ion stage is one or greater than the species will be interpreted as an atom or ion. An ion stage of zero indicates that one of the special cases listed where ***cdColm*** is described. As an example, the following will obtain the column densities of molecules and levels

```
punch some column densities “test.col”
H2   0   // the hydrogen molecule
CO   0   // the carbon monoxide molecule
C11* 0   // the J = 0 level of atomic carbon
end of column densities
```

This command can be combined with the **punch grid** command (page 154 below) to save predictions from a series of grid calculations (see page 199 below).

The **punch FeII column density** command is described on page 151 below. The **punch H2 column density** command is described on page 156 below.

14.38. punch continuum

This command is a primary mechanism for saving the predicted spectrum.

14.38.1. Lines in the spectrum

Emission lines are included in the output for all **punch continuum** commands except **punch transmitted continuum**. They are visible in the net emitted continuum. Labels giving one of the lines contributing to each wavelength are given in the third to last column in the punch output. More than one line will contribute to many wavelength cells and the last column indicates the number of lines within that cell. The line label does not give the strongest contributor to that cell. Rather it is the first line that happens to fall within that cell during the code's initial set up.

The **print continuum indices** command (page 133 above) will list the labels for all lines that enter into each cell. This provides a way to see all lines that contribute. The **print line sort wavelength** (page 136 above) can be used to find the strongest line that occurs at a particular wavelength or energy.

14.38.2. Emission line – continuum contrast

Emission lines are included in the output for all **punch continuum** commands except **punch transmitted continuum**. In nature the line to continuum contrast depends on the intrinsic width of the line. By default the lines are added to the continuum assuming that they have an intrinsic width of 1000 km s^{-1}. This can have the effect of making lines appear to be either too strong or too weak relative to the continuum, depending on the actual line width. The assumption also changes the summed total intensity of entries in the punch output file. Other line widths can be set with the **set PunchLWidth** command described on page 216 below. This issue is discussed further in the section *Observed Quantities* in Part 3 of this document.

14.38.3. Pumped contributions to the lines

Continuum pumping and fluorescence are included as excitation processes for all lines. These contributions are usually not printed as a separate quantity but will be if the **print line pump** command (page 136 above) is entered. Whether or not the pumped contribution actually adds to the observed line emission depends on the geometry. Continuum pumping increases the line emission if no related continuum absorption is seen by the observer. This will be the case if the continuum source is either not observed or not covered by absorbing gas on the observer's line of sight. If absorbing gas covers an observed continuum source then the situation is like the P Cygni problem, emission is the result of absorption and pumping may not increase the total intensity of the line at all.

The line intensity includes fluorescent excitation unless the **no induced processes** command is entered. That command is unphysical since it turns off all induced processes. You can judge how great the contribution of the pumped part of the line is by printing it with the **print line pump** command (described on page 136 above).

In general the treatment of scattering is very geometry dependent. The output produced by the **punch continuum** commands *does not* include the pumped part of the line contribution. This is correct if the continuum source is included in the beam, but is not if only the gas is observed.

14.38.4. Units of the punch output

By default, the energy units for the first column, which gives the wavelength or energy for each point in the continuum, are Rydbergs. The units can be changed to any of several energy or wavelength units with the **`units`** keyword that appears on a **`punch continuum`** command. The following keywords are recognized: **`microns, _keV, _eV_, Angstroms, centimeters`** (also **`_cm_`**), **`wavenumbers`**, **`MHz`**, and **`Rydbergs`**. Both the keyword **`units`** and one of these units must appear for the units of the energy scale to be changed.

The units of the predicted continuum depend on whether the intensity or luminosity case (see page 10 above) is used. In the intensity case continua are given as the intensity per octave $4\pi \nu J_\nu$ [erg cm^{-2} s^{-1}]. In the luminosity case they are $\nu L_\nu / 4\pi r_o^2$ [erg cm^{-2} s^{-1}] relative to the inner radius of the cloud so the monochromatic luminosity per octave is the predicted quantity multiplied by $4\pi r_o^2$.

14.38.5. Punch continuum predictions

The **`punch continuum`** command, with no other keywords, produces a file with the following information. The different contributors to the continuum are defined on page 6.

Column 1. The first column gives the photon energy in the units set with the **`units`** option (described on page 144 above). The default units are Rydbergs.

Column 2. This is the incident continuum at the illuminated face of the cloud.

Column 3. This is the transmitted incident continuum and does not include diffuse emission from the cloud.

Column 4. This is the outward portion of the emitted continuum and line emission. This includes a covering factor (discussed on page 77 above) if one was specified. The total emission from the cloud will be this multiplied by the inner area of the cloud. This does not include the attenuated or reflected portions of the incident continuum.

Column 5. This gives the net transmitted continuum, the sum of the attenuated incident (column 3) and diffuse (column 4) continua and lines. This would be the observed continuum if the continuum source were viewed through the gas. It includes the covering factor.

Column 6. This is the reflected continuum and is only predicted for an open geometry.

Column 7. This is the sum of the transmitted and reflected continua and lines. The attenuated incident continuum is included.

Column 8 and 9. Line and continuum labels indicate the lines and continuum edges that might contribute at that energy. If than one line is included in a continuum cell then the label gives the first one placed there, not the strongest line.

These labels are established when the code is set up and they do not mean that the line or continuum edge is actually present in the spectrum.

Column 10. This gives the number of emission lines within that continuum bin, divided by the ratio of the energy width of the cell to the cell's central energy, *dE/E*. So this is the number of lines per unit relative energy.

14.38.6. What is observed

Figure 10 illustrates several possible geometries. Two lines of sight to the central object are shown, and two clouds are shown. Each cloud produces both a reflected and transmitted emission component.

Three possible geometries, indicated by the letter on the figure, occur depending on how we view the central source and clouds: a) we do not directly observe the central object although we may see it by reflection from the illuminated face of a cloud, b) we observe the transmitted continuum and the outward emission from the emitting cloud, and c) we observe the unattenuated continuum directly without absorption. Column 2 gives the unattenuated continuum, and column 3 given the attenuated continuum.

There are also three possible situations for the line emission. First, we might only observe clouds that lie on the near side of the continuum source. In this case we see the "outward" line emission. Second, we might only observe clouds that lie on the far side of the continuum source. In this case we only see the "reflected" or inward component. Lastly, we might observe a symmetric geometry with reflected emission from the far side and outward emission from the near side.

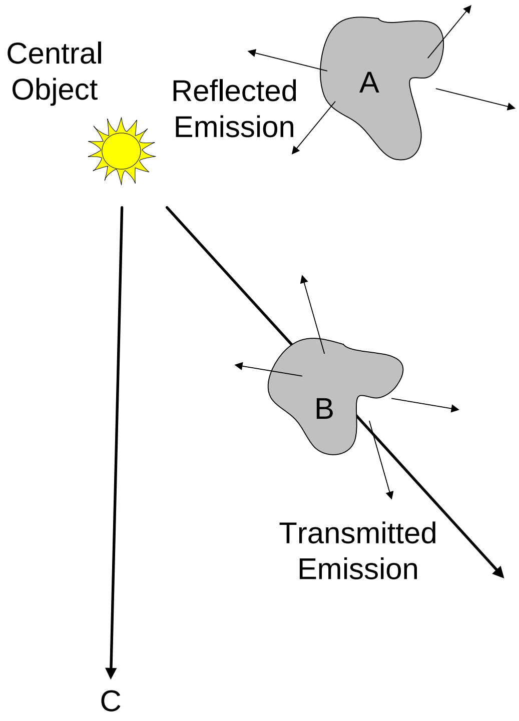


Figure 10 This figure illustrates several of the continua that enter in the calculations. ObsContin

In most cases an observer at large distance from the structure would observe *both* the central object and the cloud and would measure the quantity listed in column 5 (if only transmitted emission is detected) or column 7 (if both reflected and transmitted continua are seen). If the central object is not seen then the quantity in column 4 would be observed.

14.38.7. punch continuum bins

This punches the continuum energy bins. The first column is the center of the bin. The second column, which is nearly equal to the first, is the mean energy of the cell, weighted by the continuum shape. This has a slight dependence on the continuum shape. The last number is the cell width $\delta\nu$. The bin extends from $\nu-\delta\nu/2$ to $\nu+\delta\nu/2$.

14.38.8. punch diffuse continuum

This punches the locally produced diffuse continuous emission from the gas for the last zone. Optical depth effects are not included and the output gives the local continuum for the last computed zone. The output gives the photon energy and diffuse continuum [νf_ν erg cm^{-3} s^{-1}].

14.38.9. punch emitted continuum

The continuum emitted and reflected from the nebula is punched. The first column is the photon energy. The second column is the reflected spectrum. The third column is the outward diffuse emission. The fourth column is the total emission (the sum of the inward and outward emission). This would be the observed emission from the nebula if the central continuum source was not in the beam but clouds uniformly cover the continuum source. The last two columns are labels for lines and continua contributing at each energy. The attenuated incident continuum is not included in any of these components. All continua have units νf_ν [erg cm^{-2} s^{-1}] at the inner radius.

14.38.10. punch fine continuum [range, merge]

The code transfers the continuum on a coarse mesh, needed for speed in evaluating photo-interaction rates, and on a fine mesh, needed for automatic treatment of line overlap. The coarse continuum is the one given in output from the **`punch continuum`** command and it includes all the components shown in Figure 10 on page 145 above. The fine continuum gives a normalized attenuated incident continuum and does not include diffuse emission from the cloud. This multi-grid approach is needed to combine precision and speed. This command will output the transmission coefficient, $I_{transmitted}/I_{incident}$, for the fine continuum.

The resulting output will be huge if the entire fine continuum is punched. The command accepts a **`range`** option to limit the size of the output file. If the keyword **`range`** appears then the lower and upper limits to the range of the fine continuum must be entered in Rydbergs. The command also accepts a **`units`** option to change the units used in the resulting output. (The **`range`** option does not, at present, recognize the **`units`** option – the range must be in Rydbergs). The optional third numerical parameter gives the number of fine continuum cells to average together, again with the intent of reducing the size of the output file. The default is to average over 10 cells. If the number of cells to be combined is specified then it must be the third number on the command line, following the lower and upper limit of the range.

14.38.11. punch grain continuum

The thermal emission by grains is part of the emergent continuum. This command punches only the grain emission in the optically thin limit for the last zone. It is mainly intended as a debugging aid.

The first column gives the photon energy in the units specified with the **`units`** option. The second column gives the total emission from carbonaceous grains (including amorphous carbon and PAH's. The third column gives all emission from all constituents that are not carbonaceous. In practice this will be mainly the silicates. The last column gives the sum of the two.

14.38.12. punch incident continuum

The incident continuum, that emitted by the central object and striking the illuminated face of the cloud, will be punched. The two columns give the photon energy and the continuum νf_ν [erg cm^{-2} s^{-1}].

14.38.13. punch interactive continuum

This gives the integral of the product of the internal radiation field times the gas opacity. The results are produced for each zone and give the attenuated incident continuum, the OTS line, the OTS continuum, the outward continuum and the outward lines. The first optional number is the lowest energy in the output. If missing or zero, the lowest energy considered by the code will be used. Numbers less than 100 are interpreted as the energy in Rydbergs and those greater than 100 as the cell number.

14.38.14. punch ionizing continuum [options]

This creates a file that can be used to indicate ionization sources. If the keyword **`every`** occurs then this is punched for every zone, otherwise it is only punched for the last zone. The first column is the cell number of the C scale, so the first cell is zero. Next comes the photon energy in Rydbergs unless changed with the **`units`** option. The third column, with the header "flux", is the flux of photons within this frequency bin (*not* per unit frequency) with units s^{-1} cm^{-2}. The forth column gives the photo-interaction rate, the product of the flux multiplied by the gas opacity [cm^{-2}] and so with units s^{-1}. The next five numbers are the fractions of this photo-interaction rate due to the attenuated incident continuum, the OTS line, the OTS continuum radiation fields, and the outward lines and continua. The 10th column, with the heading "rate/tot", is the ratio of this photo rate to the total integrated radiation-field interaction rate. The next column, with the heading "integral", is the integrated cumulative interaction, the integral of the previous column over energy. This makes it easy to identify the portions of the radiation field that have the dominant interaction with the gas. The last two labels on the line indicate which lines and continua contribute at that energy.

The first optional number on the command line is the lowest energy to consider in the output. If it is missing or zero then the lowest energy considered by the code will be used. It is interpreted as the energy in Rydbergs if the number is less than 100 and as the cell number if it is greater than 100. The second optional number is the threshold for the faintest interaction to print. The default is one percent of the quantity given in the "rate/tot" column. Enter zero for this number if you want all interactions to be printed. The optional numbers may be omitted from right to left.

14.38.15. punch outward continuum

The photon energy is followed by the attenuated incident continuum, the outwardly directed diffuse continuum, the outward lines, and the sum of the two. If the **local** keyword also appears then only the outward continuum produced in the last computed zone will be punched.

14.38.16. punch raw continuum

This punches the "raw" continua. This is exactly the continuum used within the code. The first number is the photon energy. The next columns are the contents of the arrays ***flux, otslin, otscon, refcon, outcon, outlin,*** and ***condif*** at this energy. Each gives the number of photons stored in that cell with units photons s^{-1} cm^{-2} cell^{-1}. The last number is the number of lines within that cell.

14.38.17. punch reflected continuum

The reflected continuum is output if **sphere** is not set. The first column is the photon energy, the second the reflected continuum $4\pi \nu J_\nu$ [erg cm^{-2} s^{-1}] at that energy. The third gives the reflected lines and the fourth is the sum of these two. Someone who could only see the illuminated face of the cloud would observe this. The next column is the effective albedo of the cloud, the ratio of the reflected to incident continuum (the **punch total opacity** command, described on page 166 below, will give the true albedo). The last column gives the label for continuum processes with thresholds at each energy.

14.38.18. punch transmitted continuum

This saves the transmitted (attenuated incident and outward component of diffuse) continuum predicted at the end of the calculation.

This punch file can be used as part of the incident continuum in a later calculation by reading in this file with the **table read** command (see page 42 above). Three cautions apply when reading this file as an input continuum. First, if the keyword **last** does not appear on this command then the continuum from each iteration will be punched and the code will become confused when it tries to read this file. You should include the **last** option on the command since you only want results from the last iteration. Second, punch output should not be written into the same file as the input file during the second calculation. The file containing the first continuum will be overwritten if this occurs. Finally, the first two lines contain header information and they are skipped. They should not be deleted.

The line-to-continuum contrast factor ***PunchLWidth*** (see page 216 below) is not used in this command. This is to insure that lines have the correct intensity in the punch file, as needed for energy conservation. This has the effect of setting the line width to the speed of light.

14.38.19. punch two photon continuum

This punches the total two-photon continuum and is mainly a debugging aid. The photon energy is followed by the number of photons emitted per Rydberg per second, then by νF_ν. The details of two photon emission, including induced processes, are discussed by Bottorff, Ferland & Straley (2006).

14.39. punch convergence [reason, error]

These commands produce information about various aspects of the converged solution.

14.39.1. punch convergence base

The gives computed values of many quantities that are converged during a calculation. The values are given as they are at the exit to the base convergence routine. Depending on the convergence properties of the solution, there will be between only a few up to many dozens of evaluations in each zone.

14.39.2. punch convergence error

This will produce information concerning the quality of the converged pressure, electron density, and heating-cooling solution. The correct value, converged value, and percentage error, (correct-converged)×100/correct, will be produced for each zone.

14.39.3. punch convergence reason

This will punch the reason the model was declared "not converged" at the end of each iteration when the **`iterate to convergence`** command (page 99 above) is used.

14.40. punch cooling

This punches the cooling agents for each zone. The first number is the depth [cm] followed by the temperature [K]. The next two numbers are the total heating and cooling rates [erg cm^{-3} s^{-1}]. The remaining labels indicate contributors to the cooling array and the fraction of the total cooling carried by that agent. The faintest coolant punched is normally 0.05 of the total and can be reset with the **`set WeakHeatCool`** command (page 220 below).

This is mainly used for debugging and its output is not well documented. The line labels may, or may not, correspond to labels used in the main emission-line output. The code adds individual coolants to the total cooling by calling routine ***CoolAdd***. The arguments to that call include the string and a number that follows it. To discover the process for a particular label you will need to search over the entire code to find where that string occurs in a call to ***CoolAdd***. The string will be within a pair of double quotes. As an example, two coolants that might appear are **`dust 0`**, and **`H2cX 0`**. A search on the string **`"H2cX"`** (include the beginning and ending double quotes) will find the string occurring in two places, where the cooling is added with the call to ***CoolAdd*** and another place where the cooling itself is evaluated. Comments around the call to ***CoolAdd*** indicate that **`H2xC`** is cooling due to collisional excitation within the ground electronic state of H_2. A search on the string **`"dust"`** finds its call to ***CoolAdd*** with the comment that it is cooling due to grain recombination cooling.

Cooling due to the unified iso-electronic sequences is different since the label that occurs in the call to ***CoolAdd*** is generated by the routine that evaluates the cooling and does not explicitly occur in the source. The iso-electronic cooling labels begin with "IS", followed by a string indicating the process, and followed by strings giving the iso-electronic sequence and the element. Search for the start of the string but not for the element name. An example might be the string "**`IScionH H `**". The "IS" indicates that it is cooling due to an ion along the iso-electronic sequences and the two ending H's indicate that the coolant is H-like hydrogen. The string **`IScion`** occurs in the source and comments indicate that the process is collisional ionization cooling. The iso-electronic cooling strings do not include a pair of double quotes in the source since the ending double quote occurs after the element names. You would search for the string **`IScion`**.

14.41. punch charge transfer

Charge transfer recombination and ionization rate coefficients [$cm^3 s^{-1}$] for hydrogen onto heavier elements will be output. The rates will be evaluated at the temperature of the last computed zone. Rates for recombination ($\mathrm{A}^{+x} + \mathrm{H} \rightarrow \mathrm{A}^{+x+1} + \mathrm{H}^{+}$) are first, followed by the rates for the opposite ionization process. The first number is the atomic number of the species.

14.42. punch _dr_

The logic behind the choice of zone thickness will be described.

14.43. punch dynamics options

This produces some information concerning the dynamics solutions.

14.43.1. punch dynamics advection

This produces information about advection terms.

14.44. punch element *name*

This will punch the ionization structure of any element. The output will have one line per zone giving the ion fraction[37] of each successive stage of ionization. The keyword **`element`** must be followed by the element name spelled with the first four characters exactly as given in Table 9 (page 47 above).

The first number on the resulting output is the depth [cm] into the cloud. The remaining lines give the relative ionization fraction of the *n+1* possible stages of ionization where *n* is the atomic number of the element. These may be followed by some of the more abundance molecules.

If the keyword **`density`** appears on the command line then the density [cm^{-3}] will be given rather than the dimensionless fraction.

[37] Before version 96 the ionization fractions only included atoms and ions. They now include molecules. The sum of the atomic and ionic fractions will not add up to unity if a significant fraction of the element is in molecules.

14.45. punch enthalpy

The file will list the depth into the cloud, followed by the total enthalpy, and various contributors to it.

14.46. punch execution times

The code will output the zone number, the time required to compute that zone, and the elapsed time since the start of the calculation. This is intended as a mechanism to identify zones that require large amounts of work to converge.

14.47. punch FeII [options …]

This produces some information about the Fe II atom. The atom is slow and is only included when the **`atom FeII`** command (page 83 above) is given.

Both "**`FeII`**" with no spaces and "**`Fe_II`**" with a space are accepted. The following examples show the first style but both are correct.

14.47.1. punch FeII column densities

This gives the excitation energy of the levels (wavenumbers), their statistical weights, and the column densities (cm^{-2}).

14.47.2. punch FeII continuum

The pseudo-continuum of Fe II lines predicted by the large Fe II atom will be punched. See page 84 above for more details. The first number in the punch output is the wavelength of the center of each continuum band in Angstroms. The second number is the integrated intensity of Fe II emission over that band in intensity units [erg cm^{-2} s^{-1}]. This command does not have the units option so it is not possible to change the wavelength units. The Fe II pseudo-continuum is always in intensity units, even in the luminosity case.

14.47.3. punch FeII departure

The departure coefficients will be punched. This is normally only listed for selected levels. All levels will be punched if the keyword **`_all`** appears.

14.47.4. punch FeII levels

A list of the energy levels in the large Fe II atom will be produced. The first column gives the energy of the level (wavenumbers) above ground and the second column gives the statistical weight of the level.

14.47.5. punch FeII lines [faint=0.1, range 0.1 to 0.3 Ryd]

This will punch all $\sim 10^5$ lines predicted by the large Fe II atom at the end of the calculation. The upper and lower level indices are given on the physics, not C, scale, so the lowest level is one. Next is the line wavelength in Angstroms, followed by the log of the intensity or luminosity of the corresponding Fe II line. This is followed by the linear intensity relative to the line set with the **`normalize`** command. The optical depth is given in the last column. If the keyword **`short`** appears then the relative intensity and the optical depth are not punched.

Three optional numbers can appear on the command line. The first is the intensity of the faintest line to be punched. This is relative to the normalization line which is usually Hβ. The second and third optional numbers are the lower and upper limits to the range of punched lines' energy in Rydbergs. Both numbers are interpreted as logs if either is negative. These optional numbers can be omitted from right to left.

14.47.6. punch FeII optical depths

The optical depths of all lines in the large Fe II atom will be produced. The first two columns give the index of the lower and upper levels on the physics (not C) scale, the third column gives the wavelength of the transition in Angstroms, and the last column gives the optical depth.

14.47.7. punch FeII populations

The level populations [cm^{-3}] for selected levels of the large Fe II atom are punched by default. All levels will be punched if the keyword **`_all`** appears. If the **`range`** keyword appears then a pair of numbers, the lower and upper indices for the levels, will be read. The populations are per unit volume by default. If the keyword **`relative`** appears then they will be given relative to the total Fe$^+$ density.

14.48. punch FITS

This command produces photon energies and transmitted continuum into a two-column file in FITS (Flexible Image Transport System) format. FITS is a standard format used in astronomy, and endorsed by both NASA and the International Astronomical Union. The most current definition of the FITS format is by Hanisch et al. (2001). This was added by Ryan Porter and its first application is given in Porter et al. (2006).

This command is often used with the **`grid`** command (see page 199 below) which creates grids of calculations.

The following creates a FITS file with a blackbody continuum

```
blackbody 100,000K
ionization parameter -2
punch FITS "filename"
```

14.49. punch gammas

This gives the photoionization rates for all subshells of all ions for the last zone. The numbers are the element, ion, and subshell numbers, followed by the photoionization and heating rates from that subshell. The remaining numbers are the fractional electron Auger yields.

14.49.1. punch gammas element oxygen 1

If the **`element`** keyword appears then the detailed contributors to the photoionization rate for the valence shell of a particular element will be produced by calling ***GammaPrt***. The ionization stage must also appear, with 1 the atom, 2 the first ion, etc.

14.50. punch gaunt factors

This produces a table showing the free-free gaunt factors as a function of photon energy and temperature.

14.51. punch grains [options]

These commands give grain properties. Several grain species are usually included in a calculation. Often there are several size bins per grain type. These commands will print a line giving a list of the grain labels, followed by a line giving the grain radius in μm. The following lines then give the individual grain properties (temperature, potential, etc) for each size and type.

Details of the grain physics are given in Baldwin et al. (1991), Weingartner & Draine (2001), van Hoof et al. (2004), and Weingartner et al. (2006).

14.51.1. punch grain abundance

The grain abundance [g cm^{-3}] for each grain bin and the total grain abundance is given as a function of depth.

14.51.2. punch grain charge

The first number is the electron density [cm^{-3}] contributed by grains. A positive number indicates that grains where a net source of electrons so they have a net positive charge. The remaining columns print the charge of each grain size and type, in number of elementary charges per grain, for each zone.

14.51.3. punch grain continuum

See page 146 above.

14.51.4. punch grain D/G ratio

The dimensionless dust to gas ratio for each grain bin and the total grain abundance is given as a function of depth.

14.51.5. punch grain drift velocity

The drift velocity [km s^{-1}] of each grain species is printed for each zone.

14.51.6. punch grain extinction

The grain extinction at the V filter will be punched as a function of depth. This extinction only includes grains, although they should provide nearly all the extinction when they are present. The first column gives the depth into the cloud [cm], the second is the extinction [mag] at the V filter for an extended source, like a PDR, and the third number is the extinction for a point source like a star. This distinction is discussed in Sections 7.2 and 7.6 of AGN3. The extended source extinction discounts forward scattering by writing the scattering opacity as $\sigma(1-g)$, where σ is the total scattering opacity and g is the grain asymmetry factor. The quantity in the last column does not include the $(1-g)$ term.

14.51.7. punch grain H2rate

The grain H_2 formation rate is given for each size and type of grain and for each zone.

14.51.8. punch grain heating

The grain heating [erg cm^{-3} s^{-1}] is output for each zone.

14.51.9. punch grain opacity

This gives the grain opacity as a function of the photon energy. The first column is the photon energy, the second the total (absorption plus scattering) cross section, followed by the absorption and scattering cross sections. These are the summed cross section per proton for all grain species in the calculation. Column 5 is the pure scattering cross section summed over all grains and column 6 is the grain albedo. Columns 2, 4, and 6 use the scattering cross section multiplied by (1-g), while column 5 does not.

14.51.10. punch grain potential

The grain floating potential [eV] is output for each grain size bin and each zone. The grain potential is defined as

$$\varphi_g = \frac{\left(\langle Z\rangle + 1\right)e^2}{a} \tag{77}$$

where <Z> is the average grain charge of the grain size bin. In reality there is a distribution of grain charges in each bin, so this quantity does not relate to any individual grain. It is approximately the amount of energy needed to move an electron from the grain surface (after it has been lifted out of the grain potential well) to infinity, averaged over all charge states. Weingartner & Draine (2001), van Hoof et al. (2004) and Weingartner et al. (2006) provide further details.

The grain potential given here and the (average) grain charge (see **`punch grain charge`** on page 153 above) differ only by constants. It is probably best to use the latter since that quantity will be far easier to define. Refer to Weingartner & Draine (2001) and van Hoof et al. (2004) for more details.

*14.51.11. punch grain _qs_*

The photon energy is followed by the absorption and scattering *Q*s for each grain species. These are defined in Chapter 7 of AGN3.

14.51.12. punch grain temperature

The temperature of each grain species is printed for each zone.

14.52. punch grid

This is used with the **`grid`** command (see page 199 below) to create a file giving the parameters for each simulation in a large grid of calculations. This can be combined with other **`punch`** commands to create files giving the derived quantities for a large set of calculations.

The first line gives column titles. The column title for the parameters that are varies will give the first few characters of the command line for that parameter. Each of the following lines summarizes a simulation. The first two columns indicate whether the calculation aborted or had any warnings. A successful calculation will have "F" (for false) indicating no abort or warning occurred. If either of these is "T" (for true) then that simulation had major problems. You should look at the detailed output to find out what went wrong. The remaining columns give parameters for each simulation in the grid.

This command will not produce any output if the set of calculations are not done with the **grid** command.

14.53. punch heating

The code will punch the heating agents for each zone. The two columns give the depth [cm] and temperature [K]. The next two columns give the total heating and cooling rates [erg cm^{-3} s^{-1}]. This is followed by a set of labels for various heat sources and the fraction of the total heating carried by that agent. The faintest agent punched is normally 0.05 of the total and can be reset with the **set WeakHeatCool** command (page 220 below).

The heating labels will probably not correspond to any entries in the emission-line list. If the identification of a heat source is in question the best recourse is to search for the heating label over the entire code.

14.54. punch [option] history

14.54.1. punch pressure history

This follows the pressure and density convergence history.

14.54.2. punch temperature history

This follows the temperature and heating – cooling convergence history.

14.55. punch H2

Some details of the large H_2 molecule are output as a punch file. One of the following options must appear. The large H_2 atom is not included by default but is turned on with the **atom H2** command described on page 85 above.

Many studies of H_2 properties will use plots showing populations as a function of excitation energy. The slope gives a population temperature, which may be related to the kinetic temperature under some circumstances. Theoretical plots can be made using the **punch H2 column density** or **punch H2 populations** commands described below. The level energy in K, given in the punch output, is the x-axis and the column density or population in each level is the y-axis.

The **punch grain H2rate** command (page 154 above) gives the H_2 formation rate for each of the grain species included in the calculation.

14.55.1. *punch H2 column density*

This punches the column density of ro-vibrational states within the ground electronic state. This command recognizes the same options as the **`punch H2 populations`** command which is described on page 157 below.

The file begins with the total H_2 column densities in the ortho and para forms, followed by the total H_2 column density. The remainder of the file gives the v and J quantum indices, followed by the excitation energy of the level in K, the total column density in that level, and finally the column density divided by the statistical weight of the level.

14.55.2. *punch H2 cooling*

This produces a file containing heating and cooling rates [cm^{-3} s^{-1}] as a function of depth.

14.55.3. *punch H2 creation*

H_2 creation processes are given for each zone.

14.55.4. *punch H2 destruction*

H_2 destruction processes are given for each zone.

14.55.5. *punch H2 heating*

This produces a file containing the depth, total heating rate [erg cm^{-3} s^{-1}], and H_2 heating predicted by an expression in Tielens & Hollenbach (1985a), together with the heating predicted by the large model of the H_2 molecule.

14.55.6. *punch H2 levels*

This creates an energy-ordered list of the levels within X. The first column gives the energy in wavenumbers relative to the lowest level, the second gives the statistical weight, and the next two columns give the vibration and rotation quantum numbers. The sum of the transition probabilities is given, followed by the critical density of the level for each of the colliders included in the calculation.

14.55.7. *punch H2 lines*

The intensities of all significant H_2 emission lines that are produced within the ground electronic state are given. The file also gives the information needed to convert an emission-line spectrum into a level population vs excitation energy diagram.

Each line of output begins with a spectroscopic designation of the line, followed by the upper and lower electronic, vibration, and rotation quantum numbers. This is followed by the wavelength of the line in microns. The line wavelength is then printed as it appears in the output. The log of the intensity or luminosity in the line (depending on whether the intensity or luminosity case is specified), and the intensity of the line relative to the normalization line, follow. The excitation energy of the upper level of the transition in Kelvin and the product $g_u h\nu A_{ul}$ for each line are also given. This product is needed to convert intensities into excited-state column densities.

Only lines brighter than 10^{-4} of the reference line are given by default. The intensity of the faintest line, relative to the normalization line, is set with the first optional number that can appear on the command line. If the number is negative then it is interpreted as the log of the limit.

By default only lines within the ground electronic system are punched but this can be changed if the keyword **`electronic`** appears on the command line. If the keyword **`_all`** also appears then lines within all electronic systems are punched. If the keyword **`ground`** appears then only lines the ground system are punched. This is the default. If a number appears then it is the number of electronic systems to be punched, 1 for only the ground electronic state. If the number of systems is specified then it must be the second number on the line – the first being the intensity of the faintest line to print.

The following give examples. The first sets the faintest H_2 line to punch. Only lines within the ground electronic system will be produced.

```
punch H2 lines, faintest -4 “filename”
```

This sets the faintest line, and also requests all lines produced by all electronic configurations.

```
punch H2 lines, faintest -4 all “filename”
```

This example requests only lines for the lowest three electronic configurations.

```
punch H2 lines, faintest -4 electronic 3 “filename”
```

14.55.8. punch H2 populations

The level populations for the ground electronic state are given for the last computed zone. The populations are relative to the total H_2 abundance.

There are several optional parameters. The quantum numbers of the highest vibrational and rotational levels to punch can be specified as consecutive numbers on the command line. These occur in the order v then J. If no numbers occur, or if a limit that is less then or equal to zero is entered, then populations of all levels will be punched.

If the keyword **`zone`** appears then only the populations of the v=0 levels will be punched for every zone. These are all given along one long line, a format that is different from the other output options. Otherwise the populations are only punched at the end of the iteration using the output options described next.

If output is only punched for the last zone then it can be in either a triplet format, with the vibration and rotation quantum numbers followed by the population, or as a matrix, with all populations of a given vibration quantum number lying along a single row. The triplet form is done by default, and the second will occur if the keyword **`matrix`** occurs on the command line.

The **`punch H2 column densities`** command, described on page 156 above, provides similar output options but for integrated column densities.

14.55.9. punch H2 PDR

The output contains useful information regarding conditions within a PDR.

14.55.10. punch H2 rates

The output contains useful information regarding H_2 formation and destruction rates.

14.55.11. punch H2 Solomon

The output will give the total rate for photo-excitation from the ground to electronic excited states and then identify those levels which are the dominant contributor to the total rate.

14.55.12. punch H2 special

This provides infrastructure to punch debugging information. It can be easily changed to suite particular needs.

14.55.13. punch H2 temperatures

The depth [cm], 21 cm spin temperature [K], gas kinetic temperature [K], and several temperatures derived from relative populations of J levels within the H_2 v=0 ground electronic state [K], are punched for each zone.

14.55.14. punch H2 thermal

A variety of heating – cooling processes involving H_2 are given for each zone.

14.56. punch helium [options..]

14.56.1. punch helium line wavelengths

This gives wavelengths of lines from n=2 levels of He-like ions.

14.57. punch hydrogen

14.57.1. punch hydrogen 21_cm

This gives some information related to the spin temperature of the 21 cm line. The keyword is either “21 cm” or “21cm”. The level populations within 1s are determined including radiative excitation by Lα, pumping by the external and diffuse continua, collisions, and radiative decay. Several of the resulting populations and temperatures are included in the output.

14.57.2. punch hydrogen conditions

This gives the physical conditions and populations of various forms of hydrogen are given as a function of depth. The depth [cm], temperature [K], hydrogen density [cm^{-3}], and electron density [cm^{-3}] are followed by the densities of H^0, H^+, H_2, H_2^+, H_3^+, and H^- relative to the total hydrogen density.

14.57.3. punch hydrogen ionization

This gives rates for processes affecting the hydrogen ionization as a function of depth. The columns give the ground state photoionization rate [s^{-1}], the total and

Case B recombination coefficients [cm^3 s^{-1}], the predicted ratio of n(H$^+$) to n(H^0), and the theoretical ratio for the simple case. Finally, contributors to the ground state photoionization rate are produced with a call to ***GammaPrt***.

14.57.4. punch hydrogen _Lya

This produces some information related to the excitation, destruction, and escape of the Lα line of hydrogen. The optical depth from the illuminated face to the outer edge of the current zone is followed by the excitation temperature, electron kinetic temperature, and the ratio of these.

14.57.5. punch hydrogen populations

This gives the depth [cm], the densities of H^0 and H$^+$ [cm^{-3}], followed by the level population densities [cm^{-3}] for the levels in the order n = 1, 2*s*, 2*p*, 3, 4, 5, … for each zone.

14.57.6. punch hydrogen lines

The upper and lower quantum indices, the line energy, and the optical depth in the line, will be punched.

14.58. punch ionization means

The mean[38] ionization of all elements included in the calculation will be output. The format is exactly the same as the mean ionization printout produced at the end of the standard output.

14.59. punch ionization rates carbon

The total ionization and recombination rates for a specified element will be punched as a function of depth. The name of an element must appear on the command line. Each line of output will have the depth [cm], electron density [cm^{-3}], and the sink timescale for loss of particles due to advection out of the region [s^{-1}]. The remaining numbers give quantities for each possible stage of ionization of the element. For each ionization stage the set of numbers that are printed give the density of atoms in that ionization stage [cm^{-3}], the total ionization rate [s^{-1}], the total recombination rate [s^{-1}], and the rate new atoms are advected into the region [s^{-1}].

14.60. punch _ip_

This gives the ionization potentials of all shells of all ions and atoms of the 30 elements included in the code. The first row is the spectroscopic designation of the ion. Each additional row gives the subshell and ionization potential of that subshell in eV. The actual key is **`IP`** with a space to either side.

[38] Before version 96 the ionization fractions only included atoms and ions. They now also include molecules. The sum of the atomic and ionic fractions will not add up to unity if a significant fraction of the element is in molecular form.

14.61. punch Leiden

This command produces an output file designed for the comparison calculations presented in the 2004 Leiden meeting on PDR calculations (Röllig et al. 2007).

14.62. punch lines, options

This set of commands will punch some details about line formation.

14.62.1. punch lines, array

This gives the intensities of *all* lines in a form in which they can easily be plotted by other software. The first column lists the line energy in Rydbergs. The next gives the spectroscopic designation of the ion. The following two columns give the log of the intrinsic and emergent intensities or luminosities of the line. Only lines with non-zero intensity are included. All lines that appear in the printout will also appear in the resulting output file[39].

Lines energy are in Rydbergs by default. This command recognizes the **`units`** option, described on page 144 above.

14.62.2. punch lines, cumulative

This option tells the code to punch the log of the cumulative intensity of up to 100 emission lines as a function of depth into the cloud. The emission lines are specified on the following input lines and end with a line with the keyword **`end`** in columns 1-3.

The label used by Cloudy to identify each line in the main emission-line output must appear in column 1-4 of the line and the line wavelength appears as a free-format number in later columns. These must match the label and wavelength used by the code exactly. You can obtain this either from the main printout or from the output of the **`punch line labels`** command (see page 162 below).

The line labels and wavelengths are followed by the depth into the cloud and the integrated intensities of the lines [erg cm^{-2} s^{-1}] for each zone. This information can be used to follow the build up of emission lines across a computed structure.

The following illustrates its use;

```
punch lines, cumulative, “lines.cum”
totl 4861
12CO  2589m
13CO  2475m
o  3 5007
totl 3727
o  1 6300
end of lines
```

If the optional keyword **`relative`** is specified then the quantities will be given relative to the normalization line. The default is to give the intensity $4\pi J$ [erg cm^{-2} s^{-1}].

[39] In versions 90 and before of the code, only the level 1 and level 2 lines were output by this command.

The **punch lines cumulative** and **punch lines emissivity** commands use the same line array so both commands cannot be used in the same calculation.

14.62.3. punch line data

This punches some atomic data for all lines included in the line transfer arrays. It can be used to generate a table listing many lines and their atomic parameters. The code will stop after the data have been punched since it is left in a disturbed state.

The first set of lines consists of recombination lines from Nussbaumer and Storey (1984) and Péquignot, Petitjean, & Boisson (1991). For these the spectroscopic designation and wavelength are given followed by the log of the recombination rate coefficient.

The remaining sets of lines are those that are treated with full radiative transfer. The first are the "level 1" lines, those with accurate atomic collision data and wavelengths. The next "level 2" lines have many more lines and uses Opacity Project wavelengths and various g-bar approximations to generate approximate collision strengths. These are followed by the hydrogen and helium iso-electronic sequences, then the ^{12}CO and ^{13}CO lines. The H_2 and Fe II lines come last if these large atoms are included.

By default the atomic parameters will be evaluated at a temperature of 10^4 K. Other temperatures can be selected by entering a **constant temperature** command (page 103 above). The number of H-like, He-like, CO, H_2, and Fe II lines that are printed is controlled by the size of the relevant atoms when the **punch line data** command is executed.

14.62.4. punch lines, emissivity

This punches the emissivity of up to 100 emission lines as a function of depth into the cloud. This information can then be used by other codes to reconstruct the surface brightness distribution of a resolved emission-line object. The "emissivity" is the net emission $4\pi \bar{J} = n_u A_{ul} P_{ul} h\nu$ [erg cm^{-3} s^{-1}] produced at a point and escaping the cloud. This includes the escape probability P_{ul}.

The emission lines are specified on the input lines that follow the command and end with a line with the keyword **end** in columns 1-3. The label used by Cloudy to identify each line (use the **punch lines labels** command or look at the main emission-line intensity printout to obtain a list of lines) must appear in column 1-4 of the line and the line wavelength appears as a free-format number in later columns. The easiest way to obtain this information is to copy and paste the line identification and wavelength from a Cloudy output. The label and line must match exactly.

The punch output begins with emission-line labels and wavelengths. The remaining output gives the emission structure. The first column is the depth [cm] into the cloud. The remaining columns give the volume emissivity [erg cm^{-3} s^{-1}] for each line. The intensity is for a fully filled volume so the punched intensity should be multiplied by the filling factor to compare with observations of a clumpy medium.

The following illustrates its use;

```
punch lines, emissivity, “lines.str”
totl 4861
o  3 5007
totl 3727
o  1 6300
12CO  2589m
13CO  2475m
end of lines
```

The **punch lines cumulative** and **punch lines emissivity** commands use the same line array so these commands cannot be used in the same calculation.

14.62.5. punch lines, intensity [every 5 zones]

This option tells the code to punch the intensities of all lines with intensities greater than zero in the format used for the final printout (line label, wavelength, intensity). The default is for this to be done only after the last zone is computed. Results for intermediate zones can be punched if the additional keyword **every** appears. In this case the first number on the line is the interval between zones to punch, as in the **print every** command.

The punch output will have the line information spread over 6 columns. For some data base applications it would be better to have a single column of results. If the keyword **column** appears then a single column is produced.

14.62.6. punch line labels

This creates a file listing all emission-line labels and wavelengths in the same format as they appear in the main output’s emission-line list. This is a useful way to obtain a list of lines to use when looking for a specific line. The file is tab-delimited, with the first column giving the line’s index within the large stack of emission lines, the second giving the character string that identifies the line in the output, the third giving the line’s wavelength in any of several units. The line ends with a description of the line.

There are a vast number of emission lines predicted by the code and many lines will have the same wavelength. The line label can usually be used to distinguish between various lines with the same wavelength. This is seldom the case for contributions to the line however. The line index can be used to resolve this degeneracy in cases where you want to obtain a line’s intensity with a call to a routine. Routine ***cdLine_ip*** (described in the header file *cddrive.h* and also in Part 3 of this document) uses the line index to find the relative intensity and luminosity of a particular line. But note that this index is not necessarily the same in different calculations. It will always be the same for a particular set of input conditions but it depends on the sizes of various atoms and which chemical elements are used in the calculation.

Most emission lines in the code share a common structure. Each of these lines will enter the following into the emission-line stack:

```
532    H  1    6563A predicted line, all processes included
533    Inwd    6563A predicted line, all processes included
534    Coll    6563A predicted line, all processes included
535    Pump    6563A predicted line, all processes included
536    Heat    6563A predicted line, all processes included
537    H  1    4861A predicted line, all processes included
538    Inwd    4861A predicted line, all processes included
539    Coll    4861A predicted line, all processes included
540    Pump    4861A predicted line, all processes included
541    Heat    4861A predicted line, all processes included
```

The entries marked “Inwd”, “Coll”, “Pump”, and “Heat” indicate the inward fraction, the collisional and radiative pumped contribution to the line, and the line heating. All of these entries will occur in the file if the keyword long appears. By default these contributions to the line are now given so the above would appear as

```
532    H  1    6563A predicted line, all processes included
537    H  1    4861A predicted line, all processes included
```

14.62.7. punch line list [absolute]

This reads in a list of emission lines from a file and reports the predicted line intensities. It is designed as a way to obtain predictions for a subset of the lines that are predicted during a series of calculations. It is often used together with the **grid** command (see page 199 below) when doing grids of calculations or with the **time** command (see page 112 above) when following the evolution of a time-varying continuum source.

Filenames These are tricky since two filenames appear in this command. All **punch** commands have the name of an output file in double quotes. This is the first filename on the command line. The file containing the list of emission lines is within the second pair of quotes. In the following example

```
punch linelist “output.txt”  “LineList_HII.dat”
```

the punch output will go to *output.txt* and *LineList_HII.dat* contains the set of emission lines. Predicted intensities for the list of lines contained in the second file will be output into the first file.

This command works by calling routine ***cdGetLineList*** which is described in Part 3 of this document. The filename within the second pair of quotes is sent to this routine. You can build your own file and several sample files giving lists of emission lines are included in the data directory. They have names that are of the form *LineList*.dat* and are intended for different circumstances. ***cdGetLineList*** will first look for the list of emission lines in the current directory and then search the data directory.

The lines will be relative to the reference line by default. If the keyword **absolute** appears then they will be given in absolute units, erg cm^{-2} s^{-1} for the intensity case and erg s^{-1} for the luminosity case.

The output file will have the list of emission-line labels in the first line. The first column gives the iteration number and the remaining columns give the line predictions.

The ratio option If the keyword **`ratio`** appears then the ratio of adjacent lines will be output. There must be an even number of lines in the line-list file. The output will have the ratio of the intensity of the first divided by the second, the third divided by the fourth, etc. This provides a quick way to look at line ratios as a function of other parameters. The **`grid`** command (page 199 below) can produce grids of calculations. Suppose the file *linelist.dat* contains the following:

```
o  3     5007
totl     4363
```

This specifies the [O III] λλ 5007, 4363 lines. The following input script uses the grid command to predict the [O III] line ratio as a function of *n* and *T*.

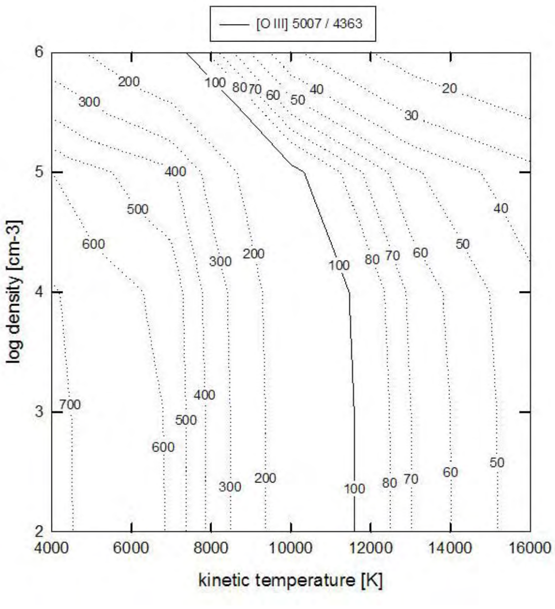
```
c produce the punch output
punch line list "O3.pun" "linelist.dat" ratio no hash
punch grid "O3.grd"
c following three commands do H and O-only, and set O
c ionization so that no O+3 is present (to prevent
c formation of 4363 by recombination).
init "honly.ini"
element oxygen on
element oxygen ionization 1 1 1 0.01
c set the continuum
blackbody 40,000K
ionization parameter -2
c next 4 commands vary Te and n
constant temperature 4 vary
grid 4000 17000 3000
hden 4 vary
grid 2 6.1 1
c must stop this constant Te model
stop zone 1
```

This produces two output files, *O3.grd* containing the densities and temperatures, and *O3.pun*, containing the ratio *I*(5007) / *I*(4363) for each density and temperature. These could be plotted to show this line ratio as a function of density and temperature, as shown in the adjoining figure.

14.62.8. punch line optical depths, limit=-2

This gives the total optical depths for all lines. By default all lines with optical depths greater than 0.1 will be included. The lower limit can be reset with the optional number that appears on the line – it is the log of the smallest optical depth to be printed. This command recognizes the **`units`** option, described on page 144 above, so the line wavelengths can be in any of the wavelength or energy units described there.

The line identification, element and ion, starts the output line, in the form used in the usual emission-line printout. Next follows the line's wavelength or energy. Finally the line's optical depth and damping constant are printed.



14.62.9. punch line RT

This produces a file containing information concerning line radiative transfer. A series of lines that specify which emission lines to produce follow the command. The line label is in columns one through four and is followed by the line wavelength. They end with a line that starts with "end".

14.62.10. punch line populations, limit=-2

This will output some information concerning the atomic parameters and level populations for all lines that are transferred.

By default all transitions with upper level densities greater than zero will be included. The lower limit to the density threshold can be reset with the optional number than can appear on the line – this is the log of the smallest population density [cm^{-3}] to be printed. This can be used to make the print out somewhat shorter. If the keyword **`_off`** appears then the limit to the smallest population to print will be turned off. All populations will be reported.

The first block of information gives an index to identify each line. This is followed by the line's label. This will usually be the spectrum, as in "H 1" followed by the wavelength, as in "1215A". The lower and upper statistical weights are next, followed by the energy of the line in wavenumbers and the *gf* value for the transition.

The population densities for each zone follow this block of information. Each line begins with the index used for that line in the atomic parameter list. This is followed by the populations of the lower and upper level of the transition [cm^{-3}].

14.63. punch map, zone 3 [range 3,999 to 4500]

This produces a map of the heating and cooling rates as a function of temperature. The details of the map are described in the description of the **`map`** command (page 110 above). The first number is the zone for the map, zero if only a map of the first zone

The optional keyword **`range`** specifies the temperature range of the map. If this option is specified then the zone number must come first and is followed by the lower and upper temperature limits to the map. Both temperatures will be interpreted as logs if the first number is ≤ 10. The keyword **`linear`** will force that interpretation. If the temperature range is specified then there must be three numbers on the line – the stopping zone number followed by the lower and upper limits to the temperature.

Normally 20 steps occur between the lowest and highest temperature in the map. The number of steps is reset with the **`set nmaps`** command (page 215 below).

14.64. punch molecules

The densities [cm^{-3}] of all molecules will be punched. The depth and the point and extended visual extinction into the cloud are given in the first three columns. The first line of the output gives header labels for the molecules.

14.65. punch opacities [total, grain, element]

This gives some of the opacity sources considered by the code. The photon energy is given in the first column and the opacities are in the columns that follow. This command recognizes the **units** option to change the energy scale (see page 144 above). One of the keywords described in the following sections must appear.

The opacities are only defined over the energy range over which the continuum source is defined. The resulting opacities will not extend to high energies for softer continua. A hard continuum such as **table agn** (page 37 above) should use used in the input stream to obtain the opacities over the full energy range.

14.65.1. punch total opacity

If the keyword **total** appears then the total opacity κ, the absorption cross section multiplied by the density of the absorber, summed over all constituents, will be punched. This has units cm^{-1}. The optical depth would be κ multiplied by a physical depth. This opacity includes all constituents, gas phase and grains, for the last computed zone, with unit filling factor. The first column is the photon energy and the second is the total opacity. The absorption and scattering opacities follow. The fifth column gives the albedo, the ratio $\kappa_s / \left(\kappa_s + \kappa_\nu\right)$. The κ's are the scattering and absorption parts of the total continuous opacity. The last column is a label indicating the ionization edge for each species included in the calculation.

14.65.2. punch grain opacity

The total grain opacity (all grain types that are included) will be punched after the last zone is calculated. Successive columns give the photon energy, the total (absorption plus scattering) opacity, the absorption opacity, and the scattering opacity. The total and scattering opacity discount forward scattering so are for the extended source case. The last column gives the scattering opacity with forward scattering included so is for the stellar case.

14.65.3. punch fine opacities range 0.7 to 1 ryd, coadd 15 cells

The code's execution time is partially set by the resolution of the continuum mesh due to the need for frequent reevaluations of opacities and rates. A very fine continuum mesh, with resolution of 1 km s^{-1} or better, is used to automatically treat line overlap. The main opacity array cannot use this resolution because single models would then have *very* long execution times. Instead, the code uses a multi-grid approach where a coarse continuum is used for most integrated quantities but a fine continuum grid is also present to handle the line overlap problem. This command will output the current contents of the fine opacity array. This only includes lines, not the continuum.

Only cells with non-zero opacity will be output. Even then, the file will be huge. If the keyword **range** occurs then the first two numbers on the command line are the lower and upper bounds to the energy range to be output. If neither is specified then the full energy range is output. The last optional number says how many neighboring cells to co-add. If no number appears then 10 is used.

The output will have energies given in Rydbergs unless this is changed with the **`units`** option. (The range is still given in Rydbergs even if the units are changed).

14.65.4. punch element opacity [name]

If neither the **`total`** or **`grains`** keywords appear then the name of an element must be specified. The keyword consists of the first four characters of any one of the 30 elements now incorporated in the code. The photon energy (eV) and total photoionization cross section (Megabarns [10^{-18} cm^{-2}]) for all stages of ionization of the specified element will be punched. A punch file name must still be specified to get past the command line parser but is totally ignored.

The photoionization cross section of each stage of ionization is punched in a series of files. The name of the file will start with the first four characters of the element's name, followed by the stage of ionization (the atom is one), ending with ".opc". Examples are **`carb1.opc`** or **`carb6.opc`**. The code stops after producing these files.

14.65.5. punch opacity figure

This version of the command creates the file needed to generate one of the figures used in Part 2 of HAZY. The output gives the energy in Rydbergs, then keV, following by the hydrogen, helium, and total gas opacities. The opacities are in units of 10^{24} cm^{-2} and have been multiplied by the cube of the energy in Rydbergs.

14.65.6. punch opacity shell 26 5 3

This punches the state-specific photoionization cross section for a subshell of any species. The first number is the atomic number of the element, the second number the ionization stage, 1 for an atom, and the third number the subshell, between 1 and 7 representing 1*s*, 2*s*, 2*p*, etc. The punch file will contain the incident photon energy in Rydbergs followed by the cross section [cm^2].

14.66. punch optical depths

This gives the total, absorption, and scattering continuum optical depths for the computed geometry. For a spherical geometry this is the optical depth from the illuminated face to the outer edge of the cloud and not the total optical depth. The photon energy is followed by the total absorption and scattering optical depths. This command recognizes the **`units`** option to change the energy scale (see page 144 above).

14.66.1. punch fine optical depths

The code's execution time is partially set by the resolution of the continuum mesh, due to frequent reevaluations of opacities and rates. For problems related to line overlap, a very fine continuum mesh, with resolution of 1 km s^{-1} or better, is used. The main continuum array cannot use this resolution because single models would then have *very* long execution times. Instead, the code uses a multi-scale approach, where a coarse continuum is used for most integrated quantities, but a fine continuum grid is also present to handle the line overlap problem. This command gives the current contents of the fine optical depth array. This only includes lines, not the continuum.

Only cells with non-zero opacity will be output. Even then, the file will be huge. If the keyword `range` occurs then the first two numbers on the command line are the lower and upper bounds to the energy range to be output. If neither is specified then the full energy range is output. The last optional number says how many neighboring cells to co-add. If no number appears then 10 cells are averaged together.

The output will have energies given in Rydbergs unless this is changed with the `units` option. The range is given in Rydbergs even if the units are changed.

14.67. punch _OTS

The line and continuum on-the-spot fields will be punched.

14.68. punch overview

This option punches an overview of the thermal and ionization structure of the cloud and is a major output mechanism for the code. The first numbers are the depth [cm], temperature [K], local heating [erg cm^{-3} s^{-1}], total hydrogen density [cm^{-3}], and electron density [cm^{-3}]. All are given as logs except for the depth.

These are followed by various ionization fractions, also given as logs of the quantity. The H_2 molecular fraction is expressed as $2n(H_2)/n(H)$. Neutral and ionized hydrogen fractions are followed by the ionization fractions for the three stages of ionization of helium, the carbon molecular fraction $n(CO)/n(C)$, the first four stages of ionization of carbon, and the first six stages of oxygen. The last column gives the visual extinction (for point and extended extinction) from the illuminated face to the current position.

14.69. punch _PDR

This gives some quantities relevant to a photodissociation region (PDR). The first column gives the depth into the cloud [cm]. The second is the total hydrogen column density [cm^{-2}]. The gas kinetic temperature follows. These are followed by the ratios of densities of H^0, $2H_2$ and $2H_2^*$ to total hydrogen, C^0 and CO to total carbon, and water to total oxygen. The next number is the (dimensionless) intensity of the UV continuum relative to the Habing background. The last columns give the total extinction in magnitudes in the *V* filter measured from the illuminated face of the cloud for a point and extended source.

14.70. punch pointers

This gives the element number, ion stage, and the shell number, for all shells of the elements heavier than helium. This is followed by the energy of the lower and upper ranges of this shell and the photoionization cross sections at these bounds.

14.71. punch physical conditions

The physical conditions as a function of depth will be punched. The depth into the cloud [cm] is followed by the temperature [K], hydrogen and electron densities [cm^{-3}], heating [erg cm^{-3} s^{-1}], the radiative acceleration [cm s^{-2}], and filling factor.

14.72. punch pressure

Various contributors to the total pressure in the gas equation of state will be punched. Pressures are given in dynes cm^{-2}. Successive columns give the following:

depth is the depth [cm] from the illuminated face to the center of the current zone.

Pcorrect is the correct pressure at the current position. This is the sum of all contributors to the total pressure. This may include, among other terms, gas, radiation, turbulent, magnetic, and ram pressure.

Pcurrent is the current pressure. It will be equal to the correct total pressure, the previous term in the output, if the pressure has been converged. The tolerance on the pressure convergence is controlled with the **`set pressure convergence`** command (see page 216 below).

PIn+Pinteg is the sum of the gas and radiation pressure due to the incident continuum evaluated at the current position. In a hydrostatic model, such as the Orion model proposed by Baldwin et al. (1991), this will be the total pressure and will be equal to the sum of the gas pressure at the illuminated face and the momentum absorbed from the incident continuum.

Pgas(r0) is the gas pressure at the illuminated face of the cloud.

Pgas is the current gas pressure.

Pram is the current ram pressure. This is only non-zero if the gas is moving, which only occurs when the wind geometry is computed.

Prad(line) is the current line radiation pressure.

Pinteg is the current integrated pressure due to attenuation of the incident continuum.

V(wind km/s) is the wind velocity in km s^{-1}. This is only non-zero for a wind geometry.

cad(wind km/s) is adiabatic sound speed in km s^{-1}.

P(mag) is magnetic pressure at the current position.

V(turb km/s) is the turbulent velocity in km s^{-1}.

P(turb) is the turbulent pressure.

conv? This is “T” if the pressure is conserved and “F” if it is not.

14.73. punch qheat

The probability distribution for the grain temperatures is punched. The first column is the grain temperature and the second column gives $dP / d\ln T$ as defined using the nomenclature of Guhatakurta & Draine (1989). Peter van Hoof added this command.

14.74. punch radius

The zone number is followed by the distance to the central object, the depth to the illuminated face of the cloud, and the zone thickness, all in cm. If the keyword **`outer`** appears then it will only write this information for the outer radius.

14.75. punch recombination [option]

14.75.1. punch recombination coefficients

Total recombination coefficients, the sum of radiative, dielectronic and three-body, will be produced for all elements in the code. These rate coefficients [cm^3 s^{-1}] are evaluated at the current electron temperature.

14.75.2. punch recombination efficiency

This gives the recombination efficiency for hydrogen, singlet helium and the helium ion.

14.76. punch results

All emission lines with non-zero intensities, and all column densities, can be saved at the end of the calculation by entering the command **`punch results last iteration`**. This is one way to save the results of a grid of models. The resulting file contains the entire input stream as well.

The resulting punch output will have the line information spread over 6 columns. For some data base applications it would be better to have a single column of results. If the keyword **`column`** appears then a single column is produced. If no keyword occurs, or the keyword **`array`** does, then the wide format is produced.

14.77. punch secondaries

The rate of secondary ionization of H^0, dissociation of H_2, and excitation of H I Lα, are given as a function of depth into the cloud.

14.78. punch source function [depth, spectrum]

14.78.1. punch source function, spectrum

The continuum source function for the local diffuse radiation field will be punched. The first column is the photon energy. The second column is the diffuse radiation field at that energy, in units of photons per second per Rydberg. Column three contains the total absorption opacity [cm^{-1}] at that energy. Column 4 contains the source function, the ratio of the diffuse field to opacity (both have the units described above). The last column gives this ratio relative to the Planck function at the local electron temperature.

The last column is a measure of the local source function relative to the local Planck function. This will generally be nearly unity for a thermal plasma close to LTE. Ground states of atoms of hydrogen and helium generally have departure coefficients greater than unity so this ratio will be less than unity at energies when their emission dominates. The helium ion can have departure coefficients much smaller than unity for nebular conditions so the source function at helium-ionizing energies can be greater than the Planck function.

14.78.2. punch source function, depth

The source function of the diffuse field at an energy slightly greater than the Lyman continuum edge will be punched for all depths into the cloud. All quantities are evaluated at the lowest energy continuum cell that lies within the Lyman continuum. The first column gives the integrated optical depth from the illuminated face of the cloud to the current position. The second is the ratio of the diffuse field (photons per Rydberg per second) to the absorption opacity. The third is the OTS continuum at this frequency, and the last is the ratio of the OTS continuum to the opacity, a photon measure of the OTS source function.

14.79. punch special

If **`special`** is specified then routine ***PunchSpecial*** will be called. This routine can be changed to fit the circumstances.

14.80. punch spectrum

This command is being developed to replace the **`punch continuum`** command described above. It works together with the **`set spectrum`** command (see page 217 below), to form a type of punch output that can be modified to suite a particular purpose. The **`set spectrum`** commands occur before the **`punch spectrum`** command, and modify the behavior of that punch command.

The units of the continuum are changed with the **`units`** option described on page 144 above.

This command is still under development and should not be used except for testing.

14.81. punch tegrid

The history of the last *NGRID* evaluations of the heating and cooling will be punched. *NGRID* is set in a header file. This is one way to evaluate the stability of the thermal solutions.

14.82. punch temperature

The radius is followed by the temperature and the derivative of the cooling with respect to temperature dC/dT. Next come the first and second spatial derivatives of the temperature with respect to depth, dT/dr and d^2T/dr^2. These derivatives set the rates of conductive heat flow and heat loss respectively.

14.83. punch time dependent

This gives some information on a time-dependent model. It is still under development, like the time-dependent physics itself.

This command is still under development and should not be used except for testing.

14.84. punch TPredictor

The code estimates the temperature of the next zone from the changes in temperature that have occurred in previous zones. This is only attempted in a constant density geometry. This output gives the old temperature, the estimated new temperature, and the final equilibrium temperature.

14.85. punch XSPEC [atable/mtable]

This command produces a file in FITS format for input into the spectral analysis program XSPEC (Arnaud 1996). This command was added by Ryan Porter and its first application is given in Porter et al. (2006).

Either **`atable`** or **`mtable`** must be specified. These keywords refer to additive and multiplicative tables respectively. This command is used with the **`grid`** command (see page 199 below) to produce grids of calculations. The files produced by this command contain predictions of each of the simulations. A file produced with **`mtable`** contains the energy bins and total optical depth, exp(-τ), from the illuminated face to the last zone of each simulation in the grid. A file produced with **`atable`** contains the energy bins and some component of the spectrum, as determined by the following options:

[attenuated/reflected] incident continuum – punches the incident continuum, the attenuated incident continuum or the reflected incident continuum;

[reflected] diffuse continuum – punches the outward diffuse continuum or the reflected diffuse continuum;

[reflected] lines – punches outward lines or reflected lines; and

[reflected] spectrum – punches the total outward spectrum or the total reflected spectrum.

The transmitted portion will be punched if neither **attenuated** nor **reflected** is included. By “reflected” we mean components escaping into the 2π sr subtended by the illuminated face toward the continuum source. If no options are specified for the **`atable`** command then the transmitted spectra will be punched. Note that the command can be specified multiple times, allowing the user to individually punch any or all of the separate components of the predicted spectra.

In the example below we specify that a blackbody is to be varied. The number on the **`blackbody`** line is ignored. The **`range`** command specifies that the log of the temperature of the blackbody will range from 4 to 6. The **`grid`** command (see page 154 above) specifies that we are calculating a regularly spaced grid with 1 dex steps between 4 and 6. In this case since we only have one parameter varied with the **`vary`** keyword, there will only be one dimension in the grid and only three simulations. Each of the two **`punch xspec atable`** commands produces a FITS format file. The first file, named *filename1*, will contain the incident continuum for each of the three simulations. The second file, named *filename2*, will contain the transmitted spectrum for each of the three simulations. The commands are as follows:

```
blackbody 100,000K vary
grid range 4 to 6 in 1 dex steps
```

```
punch xspec atable incident continuum "filename1"
punch xspec atable spectrum "filename2"
```

14.86. punch wind

The radius and depth [cm] are followed by the velocity [cm s^{-1}], total radiative acceleration [cm s^{-2}], the accelerations due to lines and continua alone, and the dimensionless force multiplier. If the keyword **`terminal`** appears then this is only produced for the last zone, otherwise it is for every zone. This option can be combined with the **`punch grid`** command (page 154 above) to save predictions from a series of grid calculations (see page 199 below).

14.87. state [_get; _put] "filename"

This command either saves or recovers the conditions computed in a previous calculation. In both cases the name of a file must appear between two double quotes. If the keyword **`_get`** appears then the file is opened for reading. It must contain the state variables for a previous iteration of the same simulation. If the keyword **`_put`** appears then the file is opened for writing and the code's state at the end of the calculation is saved in the file. If the keyword print appears on the command line then a detailed printout of the contents of the state file is produced.

This is intended as a debugging aid for dynamics simulations which require many dozens of iterations to approach a solution. It is under development and is not ready for use.

14.88. title This is a title

The argument is a title for the calculation and can be useful for organizing the models in some manner. The title is reprinted several times.

14.89. trace zone 94 [iteration 2; options . .]

This command turns on "trace" information to follow the logical flow within Cloudy. The code uses adaptive logic to control the calculation and this option provides a way to follow these internal decisions.

The trace begins *after* the zone given by the first number on the line. If the zone is zero, or if no numbers occur on the line, then the trace is turned on at the beginning of the calculation. The second (optional with default of 1) number is the iteration on which the trace should be started. It should be set to 2 to turn on the trace for the second iteration. So the command **`trace 0 2`** would start the trace at the beginning of the second iteration.

Table 15 lists the trace keywords in column 1. The four-character part of the key that must be matched is capitalized. The logical variable in Cloudy that is affected is in column 2. The purpose of each is indicated in column 3.

A string including the word DEBUG is printed when the **`trace`** command is parsed. This will not be printed if the option **`no print`** occurs on the trace command.

14.89.1. trace convergence level

This is a special form of the **`trace`** command that prints an overview of the decisions made during the calculation. The physical state of the gas is determined by nested pressure, temperature, electron density, and ionization solvers. This **`trace`** option makes it possible to view the decisions made by any of these solvers.

The code will check for one of the keywords **`pressure`**, **`temperature`**, **`eden`**, or **`ionization`**, and produce output explaining the decisions made by that solver and all higher ones. With no keyword all levels are printed. Successively deeper layers are obtained with the keywords listed in Table 14.

There are further keywords that create additional printout. The **`_OTS`** keyword will identify source of OTS fields. The **`ESOURCE`** option will identify sources of free electrons.

14.89.2. trace H-like [element name, full]

This turns on extensive printout describing the physics of one of the model hydrogenic atoms. The same code is used to compute atomic properties for all hydrogenic species. If the keyword **`full`** appears then the printout will be far more detailed. If no element is specified then this will only be for hydrogen itself. If the name of any other element appears then the printout will be for that element.

14.89.3. trace He-like [element name, full]

This turns on extensive printout describing the physics of one of the model helium-like sequence atoms. The same code is used for all helium-like species. If the keyword **`full`** appears then the printout will be far more detailed. If no element is specified then this will only be for helium itself. If the name of any other element appears then the printout will describe that element.

Table 14
Trace convergence keywords and routines

Keyword	Routine
`pressure`	ConvPresTempEdenIoniz
`temperature`	ConvTempEdenIoniz
`eden`	ConvEdenIoniz
`ionization`	ConvIoniz

Table 15
Trace Keywords and Effects

keyword	Quantity traced
BETA	OI 8446-Lβ problem
CARBon	carbon ionization equilibrium
CALCium	calcium ionization balance
COMPton	Compton heating, cooling, and ionization
CONTinuum	prints out photon arrays, pointers
CONVergence	convergence loop, no other printout
COOLants	cooling
DIFFuse fields	sum of recombination coef in DIFFEM
_DR_	choice of next zone thickness
EDEN	changes in electron density
GAUNt	the free-free gaunt factors
GRAIN	details dealing with grain treatment
HEATing	heating agents
HEAVies	heavy element balance
HELIum	helium ionization equilibrium
HELIum ATOM	Helium singlets ionization equilibrium
HELIum _IONized	helium ion ionization equilibrium
HELIum SINGlet	Helium singlets ionization equilibrium
HELIum TRIPlet	helium ion ionization equilibrium
HYDRogen	Minimal trce of the H ionization
IRON	Fe abundance, K-alpha emission
LINEes	line pointers, opacity. A’s, etc
leveln	LevelN n level atom routine
Ly BETA	Lβ - OI 8446 pumping problem
CMOLE HMOLE	Turn on either H_2 or CO network
MOLEcules	rate coefficients for molecules
NEON	recombination, ionization for neon
OPTIcal depths	inner, outer optical depths in STARTR
oPTIMizer	Steps in optimize command driver
_OTS	ots ionization rates
POINters	pointers for element thresholds
THREe body	three-body recombination rates for metals
TWO photon	induced two photon processes
WIND	Wind geometry

15. THE OPTIMIZE COMMAND

15.1. Overview

The **optimize** command and its keywords tell the code to vary one or more parameters to try to reproduce an observed emission-line spectrum, line flux or luminosity, a set of column densities, or temperatures. R.F. Carswell wrote the original code and first implemented the method in Cloudy and Peter van Hoof extended the methods as part of his thesis. Any of several minimization methods can be used obtain a best fit to a set of observed quantities. The desired emission-line spectrum, line flux or luminosity, column densities, and/or temperatures are specified by a series of **optimize** commands. A keyword **vary** can appear on several of the commands used to specify initial conditions (Table 16) to indicate which parameters are to be varied.

15.2. Commands with vary option

All commands with the **vary** option are listed in Table 16 below. The section beginning on page 183 below discusses details of some commands.

15.3. What must be specified

At a minimum the desired emission-line spectrum, a line luminosity, kinetic temperature, or a column density must be given. You also specify which parameters should be varied. These parameters are specified by a keyword **vary** which may appear on any of the commands listed in Table 16. Up to 20 parameters may be varied at a time. The quantities to be varied are actually entered as logs within the code and increments (the first steps away from the initial guess) are also logarithmic.

Several examples of the **vary** option in action are given in the *optimize_*.in* simulations in the test suite. A typical input stream follows:

```
// tell the code to vary the ionization parameter
// and hydrogen density
blackbody, 50,000K
hden 4 vary
ionization parameter -2 vary
stop zone 1
//
// the following specifies the observed emission lines, order is
// label, wavelength, intensity relative to H-beta, tolerance
optimize lines
O  3 5007 intensity =13.8 error =0.1
totl 3727 < 2.1 (only upper limit)
end of lines
//
```

This example tells the code to vary the density and ionization parameter to reproduce the observed intensities of two emission lines.

Information concerning the optimization process is fed to the code as a series of keywords on the **optimize** command. These are described next. Only one keyword will be recognized per **optimize** command.

Table 16
Commands with Vary Option

Command	Quantity varied	Min	Max	Inc.
abundances starburst	metallicity	0.001	36	0.2
blackbody	temperature	def	def	0.5
bremsstrahlung	temperature	def	def	0.5
constant temperature	temperature	def	def	0.1
coronal equilibrium	temperature	def	def	0.1
cosmic rays	cosmic ray density	def	def	0.2
dlaw	arbitrary density law	def	def	0.5
element - -	abundance of an element	def	def	0.2
energy density	energy density temp	def	def	0.1
filling factor	filling factor	def	0	0.5
fudge	first fudge factor	def	def	0.5
globule	density	def	def	0.2
grains	grain abundance	def	def	1.0
hden	hydrogen density	def	def	1.0
Hextra	Extra heating	Def	def	0.1
illuminate	Angle of illumination	0	$\pi/2$	0.1
intensity	intensity of source	def	def	0.5
ionization parameter	ionization parameter	def	def	0.5
luminosity	luminosity of source	def	def	0.5
magnetic field	magnetic field	def	def	0.5
metals	metallicity	def	def	0.5
phi(H)	photon flux	def	def	0.5
power law	see below	def	def	-
Q(H)	ionizing photons	def	def	0.5
radius	inner radius	def	def	0.5
ratio	alpha ox	def	def	0.2
set H2 Jura scale	scale factor for Jura rate	def	def	0.3
stop column density	column density	def	def	0.5
stop thickness	cloud thickness	def	def	0.5
table Draine	scale factor	def	def	0.1
table ISM	scale factor	def	def	0.2
table star Atlas	temperature	3,500	50,000	0.1
table star CoStar	temperature	18,521	53,397	0.1
table star Kurucz	temperature	30,000	50,000	0.1
table star Mihalas	temperature	30,000	55,000	0.1
table star Rauch	temperature	50,000	500,000	0.1
table star Werner	temperature	50,000	500,000	0.1
table starburst	age			0.3
turbulence	turbulent velocity	def	def	0.2 u_{turb}
xi	ionization parameter	def	def	0.5

15.4. Observed quantities

This section describes how to specify the observed properties we want to match.

15.4.1. optimize column density

This specifies a set of column densities. A series of column densities, ending with a line with the keyword **end** in columns 1 to 3, will be read in from subsequent lines. One column density is entered per line and up to 100 may be specified. Columns 1 to 4 of the column density lines must contain the first four characters of the name of the element spelled as in the output from the zone results. The first number on the line is the ionization stage, 1 indicates Atom I, 3 indicates Atom III, etc. The second number on the line is the log of the column density [cm^{-2}] and the last optional number is the relative uncertainty. It has a default of 0.05 (5 percent). A column density can be specified as an upper limit by entering < anywhere on the line.

The following gives an example of its use;

```
optimize column densities
hydrogen 1  < 17 // make optically thin in H^0 Lyman continuum
carbon 4 17.4 error =.001 // match the C+3 column density closely
silicon 3 14.6 // The Si+2 column density
end of column densities
```

Molecular and level column densities: how this command works: The label and ion that are parsed from the lines giving the column densities are simply passed to routine ***cdColm***. That routine is described in Part 3 of this document in the Chapter "Cloudy as a subroutine" and section "checking predictions". This optimization command accepts any species that ***cdColm*** recognizes. Column densities of molecules and excited states of some ions can be specified by entering an ion stage of zero and one of the strings that is described where ***cdColm*** is described. The first four characters of the label given on the input line must agree with those listed there.

The following shows some examples of optimizing molecular and state column densities;

```
optimize column densities
H-   0  < 17 // The H- column density is a limit
H2   0 17.4 error =.001 // Match the H_2 column density exactly
H2+  0 14.6 // The H2+ molecular ion
O11* 0  16.3 // This is an excited level within the O^0 ground term
end of column densities
```

Note that extra spaces were placed after the labels for the molecules to pad out the needed four-character label. The ion, the first number after the four-character label, is always zero

15.4.2. optimize, [intensity, luminosity]=36.425 [error =0.1]

This specifies the luminosity or intensity of a line. The code will try to make the predicted intensity or luminosity of the normalization line (usually Hβ and set with the **`normalize`** command) match this value. The sub-keyword is either **`intensity`** or **`luminosity`** and both have exactly the same effect. The number is the log of either the intensity or luminosity of the line in the same units as found in the third column of the final print out. The second (optional) number is the fractional error for the fit between the observed and computed values. If a tolerance is not specified then a fractional uncertainty of 0.10 is assumed.

Comments may be entered using any of the special characters in column 1 that were described on page 16 above.

The following gives some examples of its use;

```
// this will request an H beta intensity of 0.5 erg cm^-2 s^-1
// it applies to Hbeta since this is the default normalization line
optimize intensity –0.3

// the following resets the normalization line to 5007, then
// asks the code to reproduce its luminosity
normalize to “O  3”  5007
// we want a 5007 luminosity of 10^34.8 erg / s
optimize luminosity 34.8
```

15.4.3. optimize lines

This command tells the code to read a list of observed lines that it will try to reproduce. Up to 100 lines may be entered.

```
//
// the following specifies observed emission lines, order is
// label, wavelength, intensity relative to H-beta, tolerance
optimize lines
O  3 5007 intensity =13.8 error =0.1
totl 3727 < 2.1 (only upper limit)
O  3 88.33m 1.2
end of lines
//
```

One emission line is specified per line and the line must contain information in a specific order. Columns 1 to 4 list the label and is followed by the wavelength of the line. Both must match the identifications printed in the emission-line output. The code will stop if it cannot find an exact match. The third quantity is the observed relative line intensity. This will be in the same units as the relative intensities printed at the end of the calculation. Intensities are normally given relative to Hβ, but can be changed to other reference lines with the **normalize** command described on page 128 above. The last (optional) number is the relative error in the observed line. If an error is not specified then a fractional uncertainty of 0.05 (5%) is assumed. A line can be specified as an upper limit by entering < anywhere on the line.

The emission lines end with a line that has the keyword **end** in columns 1 to 3. If this end does not appear correctly then the code will continue reading lines until the end-of-file is encountered.

Comments may be entered using any of the special characters in column 1 that were described on page 16 above.

15.4.4. optimize temperature

This specifies a set of observed mean temperatures. Each of the lines that follow gives a species, ion stage, mean temperature, an error, and a specification of whether to weight the temperature with respect to radius or volume. The following is an example:

```
optimize temperature
```

```
Hydrogen  1  36,200K  volume
H2   0   150K     radius
end of temperatures
```

This behaves as does the previous commands. The "<" option is recognized. Numbers ≤ 10 are interpreted as logs of the temperature. The keywords **volume** and **radius** specify how to weight the mean temperature. The default is to weight over radius and will be used if no keyword is recognized. The label for the element must appear in the first four columns. The ion stage follows with the temperature and an optional error coming next. An ion stage of zero indicates a molecule.

This command simply copies the labels and parameters on the each line and passes them to ***cdTemp***, a routine that determines the mean temperature and is described in Part 3 of this document. That documentation describes how to request mean temperatures for various ions, molecules, and derived quantities.

15.5. Optimization methods

Two optimization methods are in Cloudy. The Subplex (Rowan 1990) method is the default.

15.5.1. optimize phymir [sequential mode] [8 cpu]

This uses Peter van Hoof's ***phymir*** optimization method (van Hoof 1997). In particular it tries to avoid being upset by the inevitable numerical noise that is present in any simulation. It has the further option of being able to run on multiple CPUs on multiprocessor UNIX machines.

Phymir by default runs in parallel mode (using more than one CPU) on UNIX systems and in sequential mode on non-UNIX systems. The keyword **sequential** switches ***phymir*** to sequential mode on UNIX systems. By default it will use all available CPUs. The command parser searches for a number on the line. If one is present this will be the maximum number of CPUs that are used simultaneously.

The continue option. The ***phymir*** method includes an option to restart the optimization. When an optimization run ends the code's state is saved as the file *continue.pmr*. The optimization can be restarted by including the command **optimize continue** along with **optimize phymir** command. In this case it does not start from scratch but re-starts using information in the file *continue.pmr* instead. The code is in exactly the same state when it continues as when it ended in the previous calculation. For instance, the first optimization may have ended because it hit the limit to the number of ionizations. If you restart an optimization with a *continue.pmr* file you will need to increase the number of iterations. The code would stop immediately, thinking it was already at the iteration limit, if you did not.

15.5.2. optimize Subplex

This uses Rowan's (1990) implementation of the subspace-searching simplex optimization method and is the default.

15.6. Controlling the optimizer

15.6.1. optimize file= "best.in"

At the end of the optimization process the derived input parameters are written into a file for later use[40]. The default filename is "**optimal.in"** but can be changed with this command. The file name must be valid for the system in use and must be enclosed in double quotes.

It is possible to use this file to do later calculations in which various quantities might be punched for plotting. Also it is generally a good idea to confirm that a single run with Cloudy does reproduce the same results as the many calls of the code made by the optimizer. The two should agree *exactly* but might not if the code became corrupted during the many calls made during the process.

15.6.2. optimize increment = 0.5 dex

Increments are the logarithmic quantities that will be added to or subtracted from the initial guess as the optimizer makes the first steps away from the initial value. The default increments preset in the code and listed in Table 16 were chosen with typical conditions in mind. It may be necessary to change these if the process is unable to identify a solution. If a zero is entered as an increment then the default increment will not be changed.

The increments entered with this command affect *only* the *previously* entered **vary** command. The following gives some examples of changing the increments.

```
hden 4 vary
optimize increments .1  // this sets .1 dex changes in hden
brems 6 vary            // increments left at default
radius 13.6 vary
optimize increments .05 // this sets changes in radius
```

15.6.3. optimize, iterations =75

This specifies the upper limit to the number of iterations to be performed. The default is 20. This command is quite similar to the **stop zone** command in that it is a fail-safe method to prevent runaway infinite loops. The optimization process should not stop because of this limit. It may be necessary to increase the limit if the process is still making progress at the end of the calculation.

The number of iterations that the optimizer needs depends on the number of parameters that are varied. Usually only one free parameter is varied during each step. To work well there must be enough iterations to allow each of the free parameters to be varied over a wide range. Make sure that this happens by looking at why the optimization process ended. If it ran out of iterations then you should check whether all of the parameters been varied over a significant range. If they have not then you should increase the number of iterations or vary fewer parameters.

[40] This replaces the **optimize punch** command, that was in versions 90 and before.

15.6.4. optimize range -2.3 to 3.9

The preset limits to the range over which parameters can be varied are indicated in Table 16. The entry *def* indicates the default limits of -1×10^{37} and 1×10^{37}.

It is sometimes necessary to establish physical limits to parameters. For instance metallicities may be limited to the range -1 ≤ log(Z) ≤ 0 by observations or physical plausibility. This command sets the bounds that the optimizer will use. The arguments are the lower and upper limit to the range of variation of the *previously* entered **vary** commands. Examples follow.

```
hden 4 vary
// the following sets limits to range of density
optimize range from 3 to 5
// There will be no range for this one
brems 6 vary
radius 13.6 vary
// this sets limits to radius
optimize range from 13 to 14
```

The optimizer does not actually know about the range limit. A residual of 10^{37} is returned if a parameter outside the allowed range is used.

15.6.5. optimize tolerance = 0.02

The tolerance is a measure of the desired fractional accuracy of the parameters that are varied and is set with this command. The default value of 0.10 should be sufficient for initial trial runs but the final values should be made lower for more precision.

15.7. Convergence criteria

Observables are placed into one of four categories – "spectrum", "column density", "temperature", and "absolute flux"(see van Hoof 1997) . For the i^{th} observable the error estimate is

$$\chi_i^2 = \left(\frac{F_i^m - F_i^0}{\min\left(F_i^m, F^0\right) \ \ \sigma} \right)^2 \tag{78}$$

where F^m and F^0 are the model and observed values and σ is the relative error in the observed value. The uncertainty σ is specified when the observed quantities are entered and has a default value of 0.10. The average of the error estimate is computed for each category. The error estimate summed over all categories is minimized.

15.8. Other optimizer commands

15.8.1. no vary

It is sometimes useful to be able to turn off the optimizer for a given input stream without having to change the (possibly many) occurrences of the **vary** keyword. If the **no vary** command is entered then the **vary** keyword on the other commands will be ignored and a single model will be computed.

The **no vary** command can also be used with the **grid** command (see page 199 below) to tell the code to ignore the **grid** command and **vary** options.

15.8.2. optimize, trace start 4

This turns on trace printout for the n^{th} time the code is called by the optimizer. Specific aspects of the trace are still controlled by the **trace** command described on page 175 above.

15.8.3. optimize, trace flow

This turns on trace to follow the logical flow within the optimizer.

15.9. Notes concerning commands with vary option

The keyword **vary** can appear on the commands in Table 16. Notes concerning these follow.

15.9.1. blackbody

It is not possible to specify the luminosity of the blackbody by using the keywords on the **blackbody** command when the **vary** option is used. It is necessary to enter the luminosity using some other command such as **luminosity** or **ionization parameter**.

15.9.2. cosmic ray background

This varies the cosmic ray ionization rate relative to its galactic background value.

15.9.3. dlaw

Up to 5 numbers may be entered on the **dlaw** command but only the first number will be varied.

15.9.4. elements

Either the absolute abundance of an element relative to hydrogen or the scale factor multiplying the abundance can be varied.

15.9.5. filling factor

Only the filling factor itself can be varied. It is possible to specify the optional power law for a radial dependence but it is not possible to vary it.

15.9.6. fudge factor

Only the first fudge factor will be varied. The rest are held constant at the initial value.

15.9.7. hden

It is possible to specify the exponent for the optional power-law density dependence upon radius or thickness. It is not possible to vary this additional parameter. Only the hydrogen density is varied.

15.9.8. hextra

No options are accepted. Only the direct heating can be varied.

15.9.9. illuminate

The angle must be given in radians.

15.9.10. intensity

It is possible to specify all of the options on the **`intensity`** command but it is only possible to vary the intensity itself.

15.9.11. luminosity

It is possible to specify all of the options on the **`luminosity`** command but it is only possible to vary the luminosity itself.

15.9.12. metals

The **`grains`** keyword can also be specified.

15.9.13. phi(H) *and Q*(H)

It is possible to use the **`range`** option but only the log of the photon number will be varied.

15.9.14. power law

The **`vary`** keyword appears in three forms, **`vary`**, **`varyb`**, and **`varyc`**. If **`vary`** appears then the first parameter, the slope of the power law, is varied. If **`varyb`** appears then the second parameter, the cutoff temperature in degrees Kelvin, is varied. If **`varyc`** appears then the last parameter, the low-energy cutoff, is varied. Only one parameter may be varied at a time.

15.9.15. punch output

It is not possible to use some of the punch output options while optimizing. Punch output is designed to save predictions so that they can be analyzed after the calculation is complete. It makes little sense to do this during an optimization run with its hundreds of calculations. After the optimization is complete, rerun the optimal simulation with **`punch`** commands included.

Most **`punch`** options will work during optimization. Those that read a series of lines to determine what quantities to output will not work. This is because the command parser is not used in its usual mode when commands are read during an optimization run.

15.9.16. radius

It is possible to specify the stopping radius or depth on the line but it is not possible to vary it. Only the starting radius is varied.

There could be a major source of confusion if the second parameter is entered and the two numbers are of the same order of magnitude. The logic used to interpret the second number is described on page 79 above. If the second number is greater than the first then it is interpreted as an outer radius; if less than, then the depth. As a result the interpretation of the second number can change while the first number is varied. It is safer to set an outer radius with the **`stop thickness`** command (described on page 126 above) rather than using the second number on this command if there is any danger of this confusion happening.

15.9.17. stop column density

All of the optional keywords (neutral, effective, etc.) are recognized.

15.9.18. stop thickness

Only one thickness can be specified.

15.9.19. table stars

Only the temperature can be varied, not the gravity.

15.9.20. table star CoStar

The first parameter on the command line will be varied.

15.9.21. table starburst

The age is varied. The code will return a large error to the optimizer if it requests an age that does not lie within the range of ages in the starburst data file.

15.10. Notes concerning the optimization process

15.10.1. Use physically motivated initial conditions

The algorithm will not be able to find a solution if one is not physically possible. For instance, an observed He II λ4686/Hβ intensity ratio of 0.5 cannot be produced by a 20,000 K blackbody no matter how many other parameters are varied (it produces no He^{+}-ionizing radiation). It is probably necessary to start with parameters in the general area of the successful model. When far from the solution, it is also a good idea to use a large tolerance (using the **`optimize tolerance`** command) to stop it from over-optimizing a bad solution.

15.10.2. Change the increment size

The initial increment will often be the largest step ever taken during the optimization process. If the initial parameters are far from the solution then it may be wise to increase the increments. Depending on the optimization method used, it may not be possible to find solutions more than one or two increments away from the initial guess. If the increments are too big it may jump over valid solutions.

15.10.3. Set physically motivated limits to the variable quantities

The optimizer driver uses brute force methods and understands surprisingly little modern astrophysics. For instance, while trying to reproduce an observed He II λ4686/Hβ intensity ratio of 0.5 by varying the temperature of a blackbody radiator, the algorithm is likely to examine the consequences of photoionization by a 100 K radiation field. Physically, it is known that He II emission only occurs for stars hotter than ~50,000 K (AGN3 section 2.5), so there is little purpose in examining temperatures lower than this. The process will converge more quickly if reasonable bounds to the range of the varied quantities are set using the **`optimize range`** command.

Table 17
Optimizer results

Method	Iterations	Density	temperature
Initial condition	-	5	4
Phymir	46	4.946	4.001
Subplex	39	5.002	4.002

This advice is dangerous, of course, since you may limit yourself to solutions close to those you anticipate. Experiments should also be performed far from the anticipated solution.

15.10.4. Don't give up!

My experience is that this process works about a quarter of the time. The problem is that the algorithm can easily home-in on a local minimum which is actually a very bad global solution. When this occurs the best idea is to restart the optimization process with a different set of initial conditions. Better yet is to start the process with parameters that give answers known to be close to the solution, although there is some danger of limiting the outcome to be what your expect. Finally, don't be afraid to use CPU time.

15.11. Other optimization methods?

Much of astrophysics involves solving the inverse problem – knowing an answer (the spectrum) and trying to deduce the question (the conditions that caused it). Optimizing a multi-dimensional function is more an art than a science. A truly robust optimization method would make Cloudy a far more useful research tool. I would be interested in learning about, and possibly adopting, other promising optimization methods. BSD-compatible license code is necessary.

15.12. The optimizer test cases

The suite of test cases that comes with the code includes scripts to drive each of the optimizers. These scripts are *optimize_*.in*. These were produced by first running the code at a hydrogen density of 10^5 cm^{-3} and a temperature of 10^4 K. The spectrum of [O II] and [O III] emission lines was taken from this calculation. Each optimizer starts at a density and temperature some distance away from this solution and tries to reproduce the spectrum. Table 17 shows the results of this test.

16. MISCELLANEOUS COMMANDS

16.1. Overview

This section describes commands that are used to disable physical processes, change the code's internal behavior, or to take care of housekeeping activities. These are not usually used.

16.2. assert commands

These tell the code a set of results that are expected. At the end of the calculation the expected and actual results are compared and an error condition is returned if the two disagree by more than an uncertainty. This set of commands is the foundation for automated testing of the code. In Lexington the full test suite is computed every night and a log is kept of all asserted results. An email warning is sent if any asserts fail. This insures the reliability of the code and guarantees that bugs are caught almost as soon as they are introduced.

If the characters "<" or ">" appear on the command line the expected result is taken as an upper or lower limit. The default is to check for equality.

The relative error is the second optional number on the line. If this is not specified then a relative error of 0.05 will be assumed.

16.2.1. assert Case B [H-like, He-like] element error

The H and He recombination emission from lower density photoionized clouds that are optically thick in the Lyman continuum may be close to Case B values (AGN3). This command uses stored tables of Case B emission coefficients to compare the code's computed emission with Case B expectations. Assuming that the cloud conditions are set up properly, and that certain physical processes are disabled, this provides a way to check the accuracy of models of some atoms.

One of the iso-sequences H-like or He-like must be specified. The default relative error can be changed by specifying a number on the line. The code will compare Case B with computed values for all lines that are included in the emission-line output and a botched assert will be declared if any of the code's predictions differ from Case B predictions by more than this error. A line will be printed that gives the mean error for the Case B comparisons.

assert Case B H-like [element] error The H-like option will compare the code's predictions with the Storey & Hummer (1995) results. An element name, any between hydrogen and oxygen, must also appear.

assert Case B He-like error This will compare the predictions with Case B predictions for He I emission given by Porter et al. (2005). The Case B values have the label "+Col" in the main emission-line printout. The element name must still appear but currently only helium itself can be tested.

The range option The keyword **`range`** tells the code to only check the asserted values over a restricted wavelength range. The wavelengths of the expected values are stored in Angstroms so the range must be given in the same units. This was added as a way to exclude the intensities of unobservable MIR – FIR lines. These lines come from higher levels in the atom and generally have a larger error due to the finite size of the model.

16.2.2. assert column [_CO_, H2…] 18.9

This checks the predicted column density for CO, H^-, H_2, H_2^+, H_3^+, H_2^g, H_2^*, HeH^+, O_2, SiO, C_2, C_3, OH, CN, CH^+, or CH. The labels must be surrounded by spaces. It is important that the log of the column density [cm^{-2}] appear *after* the label because of the 2 in **H2** or **O2**, etc.

The command accepts a **log** option to interpret the error as a log. The column density itself is always interpreted as a log.

For H_2 there is a **levels** option which tells the code to return the column density in a specific v, J level. This only works when the large H_2 molecule is included. The numbers on the line must appear in the following order: a) the 2 in **H2**, b) v, c) J, and d) log $N(H_2)$. The "wavelength" of the asserted quantity will be $100v + J$.

16.2.3. assert csupra –17.09

The secondary ionization rate is given by the variable *csupra*. This command checks the value of the secondary ionization rate. The number is the log of the secondary ionization rate [s^{-1}].

16.2.4. assert departure coefficients mean=1, error=0.04

This confirms that the departure coefficients predicted by one of the large model atoms are correct. The computed quantity is the mean departure coefficient for all levels in the model atom and is the first number on the line. The type of error represented by the second number depends on specifics. They are intended for situations close to LTE and so check that the predicted departure coefficient is within an error tolerance of unity.

One of the following keywords must appear.

assert departure coefficients, H-like helium, error=0.08 The keyword **H-like** tells the code that the departure coefficients predicted by an atom of the hydrogenic isoelectronic sequence should be checked. The name of one of the elements must also appear on the command line.

The error will be the largest single deviation from unity of any departure coefficient and is set with the second parameter on the command line. If the keyword **excited** appears then the ground state will not be included.

assert departure coefficients, He-like helium, error=0.08 This works like the **H-like** option, but for the helium-like isoelectronic sequence.

assert departure coefficients, FeII, error=0.08 The keyword **FeII** tells the code to confirm that departure coefficients predicted by the large Fe II atom are unity. The error is the standard deviation of the departure coefficients.

assert departure coefficient, hminus, error=0.08 The keyword **`hminus`** tells the code to confirm that the H^- departure coefficient is unity. The error is the deviation of the departure coefficient from unity.

16.2.5. assert depth 13.2

This checks that the cloud's thickness [cm] is equal to the expected value. The argument is always the log of the depth. The thickness is the length between the illuminated and shielded faces of the cloud.

16.2.6. assert eden 9

The number is the log of the electron density [cm^{-3}] of the last zone.

16.2.7. assert grain potential

The grain bin number is the first number on the line. Next comes the grain potential. This is linear eV and can be positive or negative. The third number is the optional error.

16.2.8. assert H2 grain rate -16.5

The number is the total rate [cm^{-3} s^{-1}] that H_2 forms on grain surfaces for the last computed zone. The number is a log if it is negative.

16.2.9. assert H2 ortho/para ratio 2.02

This checks the ratio of the ortho to para H_2 densities in the last computed zone. This is only meaningful if the large H_2 molecule has been turned on.

16.2.10. assert Htot –13.2

This checks that the local heating rate [erg cm^{-3} s^{-1}] of the last zone is equal to the expected value. The argument is the log of the heating rate.

16.2.11. assert HHeicf –0.013

This checks the helium – hydrogen ionization correction factor. The number is the linear difference between the atomic fractions of helium and hydrogen.

16.2.12. assert ionization fraction oxygen 3 –3.45, error 0.1, weight = radius

This checks the mean fractional ionization of an ionization stage of an element. An element name must appear somewhere on the line. The first number is the ionization stage, 1 for the atom, 2 for the first ion, etc. The second number is the expected ionization fraction. It is interpreted as a log if negative and as the linear ionization fraction if it is positive. The average can be with respect to radius or volume. The default is an average weighted with radius. If the keyword **`volume`** appears then the average will be weighted over volume.

If the keyword **`grid`** appears then the expected ionization fractions for a set of **`grid`** calculation will be entered. There must be one value for each grid point in a **`grid`** calculation (the **`grid`** command is described on page 199 below). The first and second numbers must be the ionization fraction for the first calculation and its error. The remaining numbers are ionization fractions for successive calculations. The same error is assumed for each.

16.2.13. assert molecular fraction H2 –3.45, error 0.1

This checks the mean molecular fraction. The label for a molecule, currently only H_2, must appear somewhere on the line. The next number is the expected molecular fraction. If this number is ≤ 0 it is interpreted as a log and as the linear ionization fraction if it is positive. The average can be with respect to radius or volume. The default is an average weighted with radius but if the keyword **`volume`** appears then the average will be weighted over volume.

16.2.14. assert itrzn <3.5

This checks the convergence properties of a calculation. The quantity is the number of iterations required to converge each zone. This is usually specified as an upper limit.

16.2.15. assert line "TOTL" 4861 < 1.01

This checks the relative intensity of a line. The string that gives the line label must appear between two double quotes and it must be four characters long. The line wavelength is the first number after the label. Both label and wavelength must appear exactly as they do in the output produced by the **`punch line labels`** command or in the standard emission-line output.

The second number is the expected intensity relative to the normalization line. It is always the linear intensity relative to whatever normalization line is set for the model.

The sub-keyword is actually "**`ine_`**" to avoid confusion with the keyword "**`linear`**" that appears on some commands. The command will not be recognized if the trailing space is missing.

16.2.16. assert line [luminosity intensity] "Q(H)" 4861 38.91

This compares the predicted and expected luminosities [erg s^{-1}] or intensities [erg cm^{-2} s^{-1}] of any line. This command functions exactly as the **`assert line`** command except that the quantity is the log of the luminosity or intensity of the transition and not the intensity relative to a normalization line.

16.2.17. assert niter < 4

This checks the number of iterations required in a calculation. This is usually an upper limit.

16.2.18. assert nothing 0

This will enter a clean assert into the output. This is used for those simulations in the test suite which have nothing to assert but are included for general testing.

16.2.19. assert nzone < 135

This checks how many zones were needed. This is usually an upper limit.

16.2.20. assert pressure error < 0.01

The number is the ratio of the standard deviation of the pressure to its mean value. It is interpreted as a log if it is negative.

16.2.21. assert pradmax 0.34

The asserted quantity is the maximum ratio of radiation to gas pressure.

16.2.22. assert temperature hydrogen 2, 4.02 volume, error 0.01

This checks the mean temperature of any species. The name of one of the elements or the keywords **`grains`** and **`H2`** are recognized. When the name of an element appears then the code will compare the computed mean temperature for that stage of ionization with the asserted value. The first number on the line is the stage of ionization, with 1 the atom, 2 the first ion, etc. The second number is the temperature, interpreted as a log if it is ≤ 10. It will be linear if the keyword **`linear`** appears. The last number is the relative error.

The code computes means weighted over radius and over volume. If the keyword **`volume`** appears then the temperature will be compared with the volume-weighted mean. The default is weighting over radius.

If the keyword **`grid`** appears then a series of temperatures will be entered. There must be one value for each grid point in a grid calculation (the **`grid`** command is described on page 199 below). The first and second numbers must be the temperature for the first calculation and its error. The remaining numbers are temperatures for successive calculations. The same error is assumed for each.

16.2.23. assert grain temperature index 2, temperature 234.

If no element name appears but the keyword **`grains`** does then the code will compare the computed and asserted grain temperatures. The first number on the line is an index giving the grain type. This index is from the order in which the grains were specified in the input stream and is given in the output. The first grain that occurs in the input stream is number 1. The second number is the temperature and is interpreted as a log if ≤ 10. The **`linear`** keyword forces smaller numbers to be interpreted as linear quantities. The optional error is the third number on the line. The temperature is always averaged over radius.

16.2.24. assert temperature at face 11,400K

This checks the temperature at the illuminated face of the cloud.

16.2.25. assert radius 18.2

This checks that the outer radius [cm] of the computed model is equal to the expected value. The radius is the distance from the center of the central object to the shielded face of the cloud.

16.2.26. assert thickness 13.2

This checks the thickness [cm] of the computed structure. The argument is always the log of the thickness. The thickness is the length between the illuminated and shielded faces.

16.2.27. assert velocity 7.6 km/s

This checks the final velocity of a wind model. The quantity is the expected final velocity in km s^{-1}.

16.2.28. table lines "LineList_PDR.dat"

This provides a way to check that the emission-line labels in any of the standard "*LineList*.dat*" files in the data directory are valid. This is actually a form of **`assert`** command since it will announce a botched assert if it cannot find any of the lines.

16.3. Introduction to the compile commands

The following subsections describe how to set up and then compile some external data files that are needed by the code. The stellar atmosphere files must be compiled if you wish to use some of the **`table star`** continua. Most of the other files are included in the code's distribution and only need to be compiled if you change the code.

The files produced by the compilation process must be accessible to the code when it is executed from other directories. This is most easily done if you place the compiled files in the code's data directory.

The **`compile`** command will be executed after the command parser is finished examining the input deck. You must specify a complete model to get past the parser's validation of the input stream. The easiest way to do this is to also include the **`test`** command in addition to **`compile`** commands.

The code stops after executing the first **`compile`** command it comes across. It will not do more than one compilation in a single run.

16.4. compile stars

Kevin Volk incorporated several large grids of stellar atmosphere continua into Cloudy in the 1990's. Peter van Hoof has generalized the treatment and made several extensions. The **`table star`** commands use these atmospheres. The data files are very large and "direct access" is used to read these files quickly. The result is that the final files are not portable although the code used to read or write them is. The process of converting the stellar atmosphere files from their original format into a form that can be read by Cloudy is referred to as compiling the stellar atmospheres.

These **`table star`** commands will only function if the atmosphere files are installed as described on the code's web site. This is only done once while installing Cloudy, although it will have to be done again if you ever change the continuum energy mesh. This step does not need to be done if you don't want to use these stellar atmospheres.

Full instructions on how to download and install the stellar continua are given on the code's web site.

16.5. compile opacities

N.B. This command does not now function and may be removed.

When the code is initialized it spends some time evaluating numerical fits to the needed opacities. This initialization time can be saved if the opacities are compiled and the resulting file placed on the path. To do this, execute the code and enter only the command **compile opacities**. The code will generate a binary file named **opacity.opc** containing the needed opacities and array indices. This file should be in the directory where the other data files are stored.

N.B. It is not really necessary to compile the opacities – the code will generate them when it starts up if the file does not exist. This may actually slow down the calculation if you are using a fast computer on a slow network.

16.6. compile gaunt factors

The code normally reads in a table of free-free gaunt factors when it initializes. This command regenerates that file. It was introduced by Ryan Porter.

16.7. compile recombination coefficients [H-like; He-like]

The code reads in a table of recombination coefficients for helium-like ions when it initializes. This command regenerates that file. It was introduced by Ryan Porter. One of the iso-electronic sequences must be specified with either keyword **H-like** or **He-like**.

16.8. compile grains

This command prepares the grain opacity files that are used by the **grains** command (page 58 above). This does not need to be done if the set of grains included in the data distribution (see Table 12 on page 59 above) are sufficient. You can create other species, with their own size distribution and refractive indices, by compiling them with this command. It is also necessary to compile the grains if you change the code's continuum energy mesh.

This is only a quick overview of the grains files. The file *vanhoof_grain_model.pdf* in the docs directory of the download includes far more information and should be consulted.

This command uses a spherical Mie code originally developed by Peter G. Martin using code written by Hansen & Travis (1974), and implemented into Cloudy by Peter van Hoof, to generate sets of grain opacities from a description of their size distribution and grain material optical properties (van Hoof et al. 2004). The set of grain opacities created by this **compile** command are then used to compute temperature, charge, drift velocity, and emitted spectrum, for each bin within the grain size distribution. The *vanhoof_grain_model.pdf* file in the data distribution subdirectory describes how to create new grain opacity files.

A grain model is specified by the optical properties of the material and by a description of the distribution of grain sizes. The optical properties are given by a file, with a name ending in "*.rfi*", giving the refractive indices as function of photon energy for the full energy range considered by the code. The grain-size distribution is specified in a separate data file with a name ending in "*.szd*". Sample refractive index and size distribution files are included in the data directory or you can create your own. In all cases the **compile** command combines the refractive index data with the size distribution to produce an opacity file (with a name ending in "*.opc*").

16.8.1. compile grains

With no options this compiles the minimum number of grain types needed for the `grains` command to function. This command must be given from within the directory that contains the data files. Examine the output to check for problems.

16.8.2. compile grain 10 bins, [filename, ism graphite]

This version of the command produces opacities of a single grain species and is used to create new types of grains. Both the optical properties and size distribution must be specified. This is done by giving keywords (to use one of the standard files located in the data distribution) or a filename (to read properties for a new species).

The number on the command line specifies the number of grain size bins to compute. If no number appears then 10 is set by default.

Table 19
Grain keywords for size distribution
*.szd

Keyword	Size distribution
0m010	0.01 micron
0m100	0.1 micron
1m000	1 micron
0n341	Small PAH, 15 C atoms
0n682	Large PAH, 120 C atoms
_ism	ISM distribution
ab08	Abel et al 2008
orion	Orion distribution

Keywords for standard data sets One of a set of keywords may be used to specify refractive index and grain size distributions. The keyword is the name of a file included in the Cloudy distribution without the filename extension.

A grain-size distribution may be specified with one of the keywords given in Table 19. The first three are single-sized distribution functions and are mainly used for testing the code. For single-sized grains the supplied number of cells is ignored since one cell is always used. These files have names that end in "*.szd*".

The keywords given in Table 18 may appear to specify a file containing refractive index information. These files have names that end in "*.rfi*".

Creating new data files If none of the keywords listed in the tables occur then a used-generated file is used. A pair of double quotes must surround the filename, as in "*name.rfi*". Name ending in "*.rfi*" are refractive index files while those ending in "*.szd*" are size distribution files. Filenames and keywords can be mixed on a single

Table 18
Grain keywords for refractive index data
*.rfi

Keyword	Grain type	Reference
ac1-amcarb	amorphous carbon	Rouleau & Martin 1991
be1-amcarb	amorphous carbon	Rouleau & Martin 1991
graphite	graphite	Martin & Rouleau 1991
grey, gray	grey grain	
_PAH	PAH	
silicate	astronomical silicate	Martin & Rouleau 1991

line as shown in the examples below.

16.8.3. Examples

```
// compile all grain types
compile grains

// only ism graphite
compile grains ism graphite

// use 20 bins for a silicate
// with Orion size distribution
compile grains 20 Orion silicate

// the grey.rfi file is the one read
// with the key grey, so the following
// is equivalent to grey ism
compile grains “grey.rfi” ism

// explicitly request the graphite.rfi
// (default with graphite) refractive index
// file, and the Orion size distribution
compile grains “graphite.rfi” “orion.szd”
```

16.9. crash [keywords]

This command should cause the code to crash and is used to confirm that the machine environment is correctly set. One of the following keywords must appear.

The IEEE standard for floating point arithmetic says to *not* throw an exception when a floating-point exception occurs. Instead the result is set the result to **`+/-inf`** or **`NaN`** (not a number) and have the calculation continue. The code will only crash if this is explicitly requested by setting compiler options or enabling traps on the CPU. The source includes logic that will do this on most platforms. Cloudy should crash on division by zero, overflow, or invalid operation. The **`zero`**, **`overflow`**, and **`NaN`** options on the **`crash`** command confirms this.

`crash zero` causes the code to divide a positive number by zero. This causes a division by zero exception.

`crash overflow` causes the code to divide a very large number by a very small number. The result will overflow.

`crash long overflow` causes the code to convert a floating number that is larger than the largest long int into a long int. Some machines may throw an exception in this case (mine does not).

`crash NaN` will divide zero by zero. This will cause an invalid operation exception.

`crash setnan` [**`float, double]`** will test that routine ***set_nanf*** sets float variables to NaN and that ***set_nan*** sets doubles to NaN. A variable is set to NaN with these routines and is then used in a multiplication.

`crash` i**`snan [float, double]`** will test that routine ***is_nan*** correctly determines whether a variable is NaN. A variable is set to NaN with ***set_nan*** then is asserted to not be NaN. The assert should fail.

crash assert causes the code to assert that a positive number is less than zero. This should cause an exception when the code is compiled in debug mode, but will have no effect when the optimization is set to a high level or if the flag -DNDEBUG is included with the compiler options. If the code does indeed crash with a failed assert then it may request that the output be posted on the web site. This is normal and only shows that the asserts are working properly.

crash bounds will cause an array to be evaluated with an index that exceeds the array bounds. In some cases the code may crash when this occurs.

There are three types of arrays within the code and keywords say which one to test. Malloc'd arrays are created from pointers by calling ***malloc*** or ***create***. Bounds errors for these types of arrays can be trapped with external tools such as ***valgrind*** (http://valgrind.org/) or ***Purify***. Declared arrays are explicitly given a size when the variable is declared in the source, as in

```
double c[5];
```

The Portland Group C++ compiler has options to check that limits are not exceeded on a declared array. Finally, the *multi_arr* class was introduced when the code migrated to C++ and can check on array bounds if the macro **BOUNDS_CHECK** is set when the code is compiled. This is done with the compiler option **-DBOUNDS_CHECK** on most compilers.

A keyword specifying the type of array to test must appear. The keyword **heap** checks an array that is produced by a ***malloc*** off the heap. ***valgrind*** or ***purify*** should catch these bounds errors. The keyword **static** will use a static array. Either keyword **stack** or **auto** will use an array created off the stack. Code generated by a bounds-checking compiler such as the Portland Group compiler should catch these errors. The keyword **multi** will check an array created from the *multi_arr* class. The two keywords **multi iter** will test an iterator in the *multi_arr* class. These should crash if the macro **BOUNDS_CHECK** is set. The **crash bounds multi iter** command does the same as the **crash bounds multi** command except that it tests access through iterators (which behave like pointers) rather than direct access to the array.

The **crash bounds** command has an optional offset to add to the array size **ARR_SIZE**. If *n* is positive then the code will access **array[ARR_SIZE+n]**. If it is negative then the code will access **array[n]**. The default is zero, that is, to access **array[ARR_SIZE]**. If either of two keywords, **_low** or **high**, occur with no number then the code will assume **n = 2** and check only the low or high bounds.

The **crash exception** command will cause the code to throw an exception. The exception should be caught by the handler in the main program.

crash undefined multiplies a valid constant by an undefined float. It has three possibilities. The keyword **static** will multiply by an undefined static variable. The keyword **stack** or **auto** will multiply by a variable created off the stack. If neither keyword occurs than the variable comes off the heap after a ***malloc***. The ideal compiler would produce code that crashed when any of these occurs.

16.10. drive fread, gaunts, pointers, ...

The `drive` command enters a special debug mode in which the program requests information and responds with deduced quantities. The specific debug mode is selected with the optional keywords, as described next. Parameters for a valid model (density, continuum, and luminosity) must still be specified. The debug mode is entered *after* the last command is specified and the input stream ends.

16.10.1. drive Case B

This option interpolates on Storey & Hummer (1995)'s calculations of Case B hydrogenic emissivity. The user enters the charge (1 for hydrogen, 2 for helium), temperature, density, and upper and lower quantum numbers, and the code returns the interpolated line emissivity. A null line exits the driver.

16.10.2. drive cdLine

The code will loop over all lines entered in the emission-line stack and confirm that ***cdLine*** can find each one.

16.10.3. drive E1

Values of exp(-x), E1(x), and E2 (x) will be printed for a range of x.

16.10.4. drive escape probabilities

This option examines calculations of escape probabilities. The user enters the log of an optical depth. The code queries three of the escape probability functions and reports the one-sided escape probabilities. The three are complete redistribution with damping wings, incomplete redistribution, and complete redistribution with only the Doppler core. A null line exits the driver.

16.10.5. drive fread

The free-format scanner will request an input line and then prints the interpreted number until a line with the number zero is entered.

16.10.6. drive gaunts

The program requests a temperature and photon energy, queries the free-free gaunt factor routine, and responds with the returned free-free gaunt factor. The original version of the gaunt factor routine was described in Hummer (1988) and Jason Ferguson extended it to include the full range of energy and temperature Cloudy needs. Ryan Porter recoded and reorganized the routine for version 96.

16.10.7. drive HyAs

The driver requests a pair of quantum numbers and responds with the hydrogenic Einstein transition probability. It queries the routine ***EinstA*** written by Jason Ferguson.

16.10.8. drive pointers

This interrogates the photon-energy array. After the continuum is generated the driver will ask for a photon energy in Rydbergs (interpreted as a log if negative) and responds with the cell array index, frequency, cell width, boundaries, and the phase space factor $2h\nu^3/c^2$. Once complete, the calculation will continue as usual.

16.10.9. drive pumping

This queries the routine ***conpmp***, which evaluates the continuum-line pumping probability at various optical depths (Ferland 1992).

16.10.10. drive starburst

The code will ask for a metallicity and will return the abundances of the elements by interpolating on Fred Hamann's grid of starburst abundances (Hamann & Ferland 1993).

16.11. eden -2

This adds free electrons to the gas. The argument is the log of the electron density [cm^{-3}]. This command is mainly intended to test the behavior of Cloudy in the limit of very low Compton temperatures. When the color temperature T_{color} ? 10^4 K the gas is almost entirely neutral and free electrons must be artificially added to test the Compton energy exchange problem in the strict TE limit. (Remember, charge conservation is a horrible thing to violate.)

Note: This command adds an extra component of electrons. The **`set eden`** command (page 211 below) sets the electron density. Both commands violate charge conservation.

16.12. fudge factors 4.59678 [12.3 34.5 958 ...]

The numbers appearing on the line can be communicated to any part of the code by calling routine ***fudge***. That routine has a single integer argument that is an index to the array of numbers entered on this command line. A call to ***fudge***(0) would return the first number[41], and in the example given above, a call to ***fudge***(1) would return the value 12.3. Up to ten numbers can be entered on the command line.

This command is used to pass numbers to temporary or trial parts of the code. Routine ***fudge*** is a permanent part of Cloudy and a warning is given at the end of the calculation if this function is evaluated. The code will stop if the index to the array of stored values exceeds the number of values entered. Extra numbers are simply ignored.

The code will abort if ***fudge*** is asked to return a parameter that was not defined. For instance, if the command line reads

```
fudge 4.0
```

then ***fudge***(1) does not exist and the code will terminate.

[41] In version 90 and before the array index was on the Fortran scale, so fudge(1) returned the first number. The array index is now interpreted on the C scale, so the first number is fudge[0].

fudge will return the number of parameters entered on the command line if it is called with a negative argument. The following code fragment shows how to check on the number of parameters and only then evaluating *fudge*

```
if( fudge(-1)>0 )
    factor = fudge(0);
```

16.13. grid lower limit, upper limit, increment

The **grid** command varies some of the input parameters to compute a grid of models. It is actually a form of the **optimize** command and uses much of the same code. It was added by Ryan Porter and its first use was described in Porter et al. (2006).

Parameters for those commands with the **vary** keyword (see Table 16 on page 177 above) can be varied within a grid. Each command with a **vary** option must be followed by a **grid** command. The value entered on the command with the **vary** option is ignored but must be given to satisfy the command parser.

The **grid** command line must have three numbers. The first and second are the lower and upper limits to the range of variation. The last number is the value of the increment for each step. This behaves much the same way as a *do* loop in Fortran or a *for* loop in C. The following varies the blackbody temperature over a range of 10^4 to 10^6 K with three points.

```
C the blackbody command with vary option, the 100,00K is needed to
c get past the command parser, but is otherwise ignored
blackbody 100,000K vary
c this varies the blackbody temperature from 1e4 to 1e6 K with 1 dex
c steps, so that 1e4K, 1e5K, and 1e6K will be computed
grid, range from 4 to 6 with 1 dex increments
```

The following is a 2D grid in which both the ionization parameter and metallicity are varied. There will be five values of the ionization parameter and three values of the metallicity computed.

```
ionization parameter -2 vary
grid range from -4 to 0 with 1 dex steps
metals 0 vary
grid range from -1 to 1 with 1 dex steps
```

Grid output options Several **punch** output options were developed to retrieve information from **grid** runs. The **punch FITS** command (see page 152 above) will generate FITS files for input into XSPEC (Porter et al. 2006). The **punch grid** (page 154 above) and **punch line list** (page 163 above) commands save the grid points and emission-line intensities.

When computing a grid the default is for punch files to not overwrite results of previous iterations (to not "clobber" themselves). The default is for punch files to overwrite one another when the **grid** option is not used. The **clobber** option on the **punch** command controls this behavior and is described on page 139 above.

The **no vary** command (see page 182 above) can be used to ignore all occurrences of the **grid** command and **vary** option in an input stream.

The **repeat** option on the **grid** command causes the expected number of grid steps to be computed but the initial value of the variable is not incremented. This is mainly a debugging aid.

16.14. init ["c84.ini", path]

This reads a set of commands from an initialization file. Frequently-used commands can be stored in this file and easily accessed. Common uses of this command are described on page 17 above.

There is no limit to the number of commands that can be in this initialization file other than the total limit of 4000 command lines that is intrinsic to the code. Only one **init** command can appear in a single input stream.

The default name for the initialization file is *cloudy.ini*. This will be used if no double quotes occur on the command line. Other file names are specified by including a file name within a pair of double quotes as in "*special.ini*". The name can be any name allowed by the operating system in use.

The code will look for the initialization file in the local directory first and then in the data directory as set with the path. The code will check on the path first if the keyword **path** occurs on the **init** line.

The data directory includes the *ini* files that are used in the test suite. They were set up with particular applications in mind. They may or may not be appropriate for your purpose. Please review the contents of these files before using them.

16.15. no . . .

It is possible to disable physical processes as a test of their importance. If a physical process is turned off then a flag is set to indicate that the treatment of a physical process has been disabled.

A warning will be printed at the end of the calculation as a reminder that the results of the calculation are not to be trusted. This warning will not be printed if the four-character keyword **(OK)** appears on the command line. The parenthesis is part of this keyword.

16.15.1. no advection [H-like, He-like, ...]

This turns off the effects of advection on the ionization, recombination and energy of the gas. Keywords make it possible to turn off these terms for only certain parts of the calculation. The **metals** option will turn off the effects of advection on the ionization of any species not treated as one of the iso-electronic sequences. **Cooling** will turn off thermal effects of advection.

16.15.2. no Auger effect

This turns off the Auger effect. Inner-shell ionizations will eject only one electron.

16.15.3. no buffering

Programs produce output by first writing into a buffer. Information is written to disk once the buffer is nearly full. If a C program crashes before this buffer is "flushed" the information within the buffer will be lost. This poses a problem if the printout generated just before the crash is needed for debugging. The **no buffering** command will redirect the standard output to *stderr* which is not buffered. **Punch** commands also have a **no buffering** option to turn off file buffering for the files they create.

On most systems *stderr* can be directed to a file by redirection of 2 as in the following example

```
cloudy.exe < sim.in > sim.out 2>sim.err
```

16.15.4. no charge transfer

This turns off all charge transfer interactions.

16.15.5. no collisional ionization

This turns off collisional ionization from ground states of all atoms and ions.

16.15.6. no Compton effect

This command turns off Compton heating and cooling of free electrons and Compton recoil ionization of bound electrons. Electron scattering opacity *is not* turned off.

16.15.7. no CTHeat

This turns off heating due to charge transfer. Kingdon & Ferland (1998) describe the process.

16.15.8. no diffuse line pumping

The diffuse continuum produced by gas within the cloud is included as a general line-excitation mechanism. This turns it off and is useful as a check on the importance of the process.

16.15.9. no FeII pumping

This turns off H I Lα pumping of Fe II.

16.15.10. no file opacity

The code can generate a file of stored opacities with the **compile opacity** command. This file will be used to generate the opacities in later calculations. The **no file opacity** command tells the code to ignore this opacity file even if it exists.

16.15.11. no fine structure line optical depths

Fine structure lines, such as the ^3P 52, 88 μm lines of [O III], can become optically thick under certain high-luminosity conditions (see, for example, Rubin 1983). They can absorb the incident continuum and be a significant heating source for photodissociation regions (Tielens and Hollenbach 1985a). Radiative transfer effects, including stimulated and maser emission, are fully treated for all lines. This turns off optical depths and line transfer for fine structure lines by setting the line opacity to zero.

This command does not turn off line heating - which will then be maximized since the lines will remain optically thin. The **`no induced processes`** command (described 203 below) turns continuum pumping off for all lines and should be included to disable heating due to line absorption of the continuum.

The line transfer arrays are permanently injured by the **`no fine structure`** command. Subsequent runs with the same core load in a grid will still have the line optical depths disabled.

16.15.12. no fine opacities

The code uses a fine continuum and opacity grid to automatically account for line overlap. Figure 20 of Shaw et al. (2005) shows an example of this fine mesh. Multi-grid techniques are used to propagate this fine mesh back onto the coarse mesh that is used to evaluate photo rates. This fine grid can be turned off using this command.

16.15.13. no free free

Free-free heating, cooling, and emission are turned off with this command.

16.15.14. no grain [process]

This series of commands disables various processes involving grains.

no grain electrons This turns off the effects of grain charging, either negative or positive, on the overall charge balance in the gas. This violates charge conservation.

no grain gas collisional energy exchange. Collisional energy exchange between grains and the gas is treated as in van Hoof et al. (2004) and Abel et al. (2005). This processes acts to bring the grains and gas toward the same temperature. The two temperatures will be equal if collision energy exchange is fast. Often the gas is hotter than the grains in the H^+ region and the process heats the grains and cools the gas. In fully molecular regions typically the reverse is true as the remaining continuum is very ineffective in heating the gas, but can still heat the grains. This command disables this physics.

no grain molecules Condensation of molecules onto cold grain surfaces was added by Nick Abel and is treated using the formalism outlined by Hasegawa et al. (1992) and Hasegawa & Herbst (1993). This turns off that process.

no grain neutralization Ions can become neutralized or ionized, by several stages of ionization, following a collision with a grain. Van Hoof et al. (2004) describe the treatment of these collisions. It is partially based on Draine & Sutin (1987)'s description of Coulomb interactions between the grains and gas. The effects of grain neutralization upon the ionization balance of the gas are turned off with this command although grain charging is still computed. This is not self consistent.

no grain physics This turns off all grain physics. The only remaining effect of grains is their continuous opacity. The resulting simulation will be much faster but incorrect. This is only intended to provide a method to do quick and dirty calculations. The spectrum emitted by the grains is not calculated so this command violates energy conservation.

no grain qheat This turns off quantum heating for all grain species.

no grain x-ray treatment This turns off the extensive treatment of inner shell x-ray processes within grains. This makes the X-ray physics more like Weingartner & Drain (2001).

16.15.15. no induced processes

This turns off induced recombination and its cooling, stimulated two-photon emission and absorption (Bottorff et al. 2006), continuum fluorescent excitation, and stimulated emission of all lines.

16.15.16. no ionization reevaluation

This tells the code to not constantly reevaluate the ionization rates. This option can only be set when constant density is assumed.

16.15.17. no line transfer

This turns off line transfer for all lines except the Lα transitions of the species treated with the iso-sequences. This is the approximation made in most codes designed to consider classical nebulae and may be appropriate in some cases. This command also turns off line radiation pressure.

16.15.18. no Lya 21cm pumping

Pumping of the 21 cm line by Lα is treated as in Deguchi & Watson (1985). This turns off the process. All three keywords must match.

16.15.19. no OTS [options]

no Lya OTS This turns off H I Lα OTS rates.

no HeII OTS This turns off He II Lα and recombination continua OTS rates.

no line OTS This turns of all line OTS rates.

16.15.20. no level2 lines

This turns off the large block of Opacity Project ("level 2") lines. This will cut the execution time by roughly 30%.

This should only be done in exploratory "quick look" calculations. The lines should be included for final results. These lines should not be disabled at higher densities since they may carry a large fraction of the cooling as the cloud approaches the black-body limit. They are important in UV photoexciting excited levels within split ground terms like O I* or C II*. Excited state column densities will not be predicted if the level 2 lines are disabled.

16.15.21. no molecules[H2 CO]

Cloudy does a molecule formation network that is close to today's state of the art (Abel et al. 2005; Röllig et al. 2007). The **`no H2 molecules`** or **`no CO molecules`** commands will turn off only the H_2 or CO parts of the network. There must be spaces to either side of the **`H2`** or **`CO`** keywords.

16.15.22. no on the spot

This turns on all ground-state recombination coefficients and turns off ionization by helium resonance lines. This last variable is then used to deduce the ionization efficiency of lines and continua.

16.15.23. no opacity reevaluation

Opacities are normally reevaluated every time the cooling function is reevaluated. When this is set opacities are only evaluated one time per zone.

16.15.24. no outward [options]

no outward lines This turns off the outward-only (Tarter 1967) contribution by lines.

no outward continuum This turns off the outward-only contribution by continua.

16.15.25. no photoionization

This turns off photoionization of the ground states of all elements. It is designed to test the code in the collisional-ionization equilibrium limit.

This command can cause problems. Several iso-sequences are treated as full multi-level atoms. This includes all processes that affect internal excitations. The level-populations solver may have difficulty in finding a solution when photoionization is turned off with this command but the gas is very weakly collisionally ionized. Often internal continuum pumping of the Lyman lines will dominate excitations. When these radiative terms overwhelm the collisional-ionization term the ionization rates out of the ground state may underflow. In this case the solver will find negative level populations and the code will stop announcing a catastrophic failure. One solution is to turn off continuum pumping, with the **`no induced processes`** command, described on page 203 above. Only do this if the calculation fails.

16.15.26. no radiation pressure

This command turns radiation pressure completely off. Radiation pressure due to trapped lines will be counted in the total pressure when the **`constant pressure`** option is used. The default is for a constant-density model. Radiation pressure is not included if constant gas pressure is specified.

16.15.27. no recoil ionization

This command turns off Compton recoil ionization. Compton heating and cooling of free electrons is included, but this is the only remaining thermal effect of electron scattering. Bound-electron scattering opacity is still included when this command is issued.

16.15.28. no scattering opacity

See page 99 above.

16.15.29. no secondary ionizations

This command will turn off the effects of knock-on supra-thermal electrons. Normally these are treated as in Spitzer & Tomasko (1968), Bergeron & Collin-Souffrin (1971), Shull (1979), Shull & van Steenberg (1985), Xu & McCray (1991), and Dalgarno, Yan, & Liu (1999). This command will make X-rays 100% effective in generating heat and produce no secondary ionizations or Lα excitations.

16.15.30. no Stark broadening

Stark broadening (important for densities larger than ~10^{10} cm^{-3}) is treated for hydrogen lines using the formalism described by Puetter (1981). This turns Stark broadening off.

16.15.31. no TePredictor

The code tries to predict the temperature of the next zone for constant density calculations. This stops the predictions from being used.

16.15.32. no static opacities

This forces all opacities to be reevaluated constantly within each zone. The default is to only evaluate minor opacities one time per zone.

16.15.33. no three body recombination

This turns off three-body recombination for the heavy elements that are treated as equivalent two-level systems. Three-body recombination for atoms and ions of the isoelectronic sequences is turned off by turning off collisional ionization (its time reversal) with the **`atom H-like collisional ionization off`** command (page 88 above) or the **`atom He-like`** command (page 92 above).

16.15.34. no times

This stops the code from printing execution times. Turning this off will allow exact text comparisons of results between models run at different times or on different machines.

16.15.35. no UTA ionization

This turns off ionization by absorption of inner-shell lines.

16.15.36. no vary

This command turns off the **`vary`** option set on various optimization commands. For a further discussion see page 182 above where the optimization driver is discussed in more detail.

16.16. set commands

These commands change internal variables used by Cloudy. These are mainly intended for testing and are not normally used.

16.16.1. Convergence criteria

These commands change the convergence criteria. The error in the heating-cooling balance is set with the **`set temperature convergence`** command (page

219 below). The error in the electron density is set with the **`set eden convergence`** command (page 211 below). The error in the local pressure is set with the **`set pressure convergence`** command (page 216 below). In cases where the code is having trouble converging the **`set presioniz`** command (page 215 below) will limit the number of ionization evaluations before declaring a failure.

16.16.2. set 12C13C -3.2

This sets the ^{12}C/^{13}C abundance ratio. The default is 30. If the number is negative or the keyword **`_log`** appears then the number is interpreted as the log of the ^{12}C/^{13}C ratio. It is the linear ratio otherwise. The code currently predicts the ^{13}CO rotation spectrum and the intensity of ^{13}C III λ1910 (Clegg et al. 1997) using this ratio. The code does not now solve for ^{12}C and ^{13}CO abundances and ionic fractions but rather assumes that the ratio ^{12}CO/^{13}CO and the ^{12}C^{+2}/^{13}C^{+2} ionization fractions are equal to ^{12}C/^{13}C.

The ^{12}C/^{13}C ratio depends on both location in the galaxy and age. It is ≈90 in the solar system (Anders & Grevesse 1989) and reflects the galactic value when the sun formed. The value toward the Galactic center is about 20 increasing to ≈77 at the solar radius (Wilson & Rood 1994). The default value of 30 is a compromise.

16.16.3. set assert [options]

There are very different meanings of the word ''assert'' here. The following commands apply to different types of asserts.

set assert fpt The first is a macro in the C / C++ languages that makes it simple to check that a calculation is sane. If the code is compiled with C language asserts enabled then internal sanity checks will be performed. They are not done when the code is highly optimized. This command will cause the code to abort when an assert is thrown. This can be caught if the user chooses to write code to do so..

set assert scientific notation The second asserts are commands that tell the code what value for a predicted quantity to expect. These are part of the test suite and allow automatic testing of the code's results. This command causes the printed asserted values to be printed in scientific notation rather than a float format. The **`assert`** command is described on page 187 above.

16.16.4. set atomic data [options ...]

This allows certain choices of atomic data sets to be specified in the input script. One of the keywords **`_ion`** or **`molecule`** must appear. If **`_ion`** appears then the name of an element and an integer giving the ionization stage, with 1 for the atom, 2 for the first ion, etc, must be given. If **`molecule`** appears then the name of a molecule must appear.

One of the keywords **`_CS_`**, **`_DR_,`** or **`_AS_`** (with a space before and after the two letters) must appear. These indicate whether collision strengths, dielectronic recombination rates, or transition probabilities are to be set.

The remaining options depend on the particular application. The following describe the choices currently implemented.

set atomic data ion oxygen 2 As - *Transition probabilities for [O II].* NIST recommends values from Zeippen (1987). Observational papers (Blagrave, Martin, & Baldwin 2006, Esteban et al. 2004; Wang et al. 2004) indicate that the Zeippen (1982) values are better. The keywords **old** and **new** choose which value. The default is the old values as suggested by observations.

set atomic data ion sulphur DR - *sulphur dielectronic recombination rates*. Reliable dielectronic recombination (DR) rates do not now exist for low stages of ionization of S at photoionization temperatures. The relative [S III] / [S II] ratio is an important diagnostic indicator of conditions in many nebulae. This ratio depends on the DR rates chosen. This command changes the DR rates assumed for the lowest four ionization stages of S. The default, which can also be set with the keyword **_mix**, is to use the larger of the Badnell (1991) or guessed rates. The keyword **pure** says to use only the Badnell rates. The keyword **scale** says to use scaled oxygen DR rates. In this case one to four scale factors, one for each ionization stage, will be parsed off the command line. If fewer than four numbers occur then the last number entered will be used for the missing scale factors. The DR rate for ions of S will be equal to the DR rate for the same ionization stage of O multiplied by its scale factor.

set atomic data molecule cs H2 H collisions – sets collision rates for H_2 – H^0 collisions. There are two data sets. The default is **2007** and uses the rates given by Wrathmall et al. (2007). The **1999** option uses the rates given by Le Bourlot et al. (1999).

set atomic data molecule cs H2 He collisions – sets collision rates for H_2 – He^0 collisions. There are two data sets. The default is **ORNL** and uses the rates given by Lee et al. (2008). The **Le Bourlot** option uses the rates given by Le Bourlot et al. (1999).

16.16.5. set charge transfer -11.5

This command establishes the coefficient in the statistical hydrogen charge transfer rate coefficients used for species more than four times ionized (Ferland et al. 1997). If the number is negative then it is assumed to be the log of the coefficient, if zero then this estimate is turned off, and if positive the number is the coefficient itself. It is stored as the variable ***HCTMin*** and has the default of $1.92\%10^{-9}$ cm^3 s^{-1}. This is used to set a rate coefficient of ***HCTMin*** % *q* where *q* is the excess charge of the heavy element.

16.16.6. set chemistry

This changes some aspects of the chemistry network.

set chemistry Federman [ON , OFF] This determines whether the rate coefficients derived by Zsargó & Federman (2003) are used. Their chemical network consists of a small subset of reactions important to the formation of CH, CO, HCO^+, CH_2^+, and CH_3^+ in regions with large amounts of CH^+. The default is "**ON**", that is, to use these rates instead of UMIST in the reaction network. If **OFF** is specified then UMIST rates are used.

set chemistry non equilibrium This uses the chemical model of Federman et al. (1996) to examine the effects of nonthermal chemistry on diffuse cloud chemistry. This command uses an effective kinetic temperature at which a chemical reaction proceeds that is caused by ion / molecule slip when turbulence in present. The effective temperature is given by

$$T_{eff} = \frac{3}{2}kT + \frac{1}{2}\mu\Delta u_{turb}^{2}$$

where k is Boltzmann's constant, T is the gas kinetic temperature, μ is the reduced mass of the two reactants, and Δu_{turb} is the turbulent velocity. Zsargó & Federman (2003) summarize the physical mechanism of non-thermal chemistry as:

> "The origin of the nonthermal motion is assumed to be the result of the propagation of Alfvén waves, constantly entering the cloud from the intercloud medium. The dissipation of these waves is concentrated primarily in a diffuse cloud boundary layer, the transition zone between the cloud and the intercloud medium."

The effect of T_{eff} is to increase the rates of those reactions which have a strong exp(-c/T) temperature barrier. This command primarily effects the formation of CH^+ (the abundance of which cannot be explained by equilibrium chemistry models) by eliminating the temperature barrier for the $C^+ + H_2 \rightarrow CH^+ + H$ formation channel, allowing CH^+ to form. The formation of CH^+ has trickle down effects on the predicted abundances of other molecules, such as CH, C_2, CN, and OH (see equation 7 & 8 of Zsargó & Federman 2003). This option was added by Nick Abel. The keyword can be **non equilibrium** or **non-equilibrium**.

set chemistry non equilibrium neutrals [ON , OFF] If the option **neutrals off** is also included then T_{eff} will equal T for all neutral-neutral reactions, so non-equilibrium chemistry is not included for these species. The physical assumption is that neutrals are not coupled to the magnetic field and therefore do not experience the effects of nonthermal chemistry. This was used by Federman et al. (1996) to explain low OH abundances in regions with high CH^+, such as ξ Per. By default, neutral-neutral reactions are included in the non-equilibrium chemistry.

set chemistry proton elimination [ON , OFF] In "proton elimination" reactions, an atom-molecule non-charge transfer reaction leads to the formation of either H or H^+. An example is C^+ + OH which leads to either CO + H^+ or CO^+ + H. Huntress (1977) states that the energetics of the reaction makes the H^+ formation channel highly unlikely. This command sets the rates of these reactions leading to H^+ (which currently only includes the example) to zero. By default, proton elimination is included.

16.16.7. set collision strength averaging on

This controls whether the l-mixing collision strengths used for hydrogenic levels are evaluated at kT (the default) or are an average over the thermal Maxwellian. If the keyword **on** appears then averaging will be done – this is very slow due to the large number of levels and evaluations involved. Tests show that the default, the evaluation at a single energy of *kT*, is significantly faster and produces very similar predictions.

16.16.8. set continuum options

set continuum resolution 0.1 This changes the resolution of the coarse continuum energy mesh by a constant scale factor. The resolution of the continuum mesh as a function of energy is defined by the data file *continuum_mesh.ini*, which is located in the data directory. Permanent changes to the continuum resolution should be made there. This command allows the continuum mesh to be changed by a temporary scale factor. The number on the command line multiplies the resolution contained in the data file. Factors less then unity make the cells smaller, for higher resolution, while factors greater than unity make the resolution coarser. For instance, an entry of 0.1 would make the resolution ten times finer or the resolving power ten times greater. If the number is less than zero it is interpreted as the log of the resolution scale factor.

This was originally added so that the entire continuum resolution could be improved by large factors when running some of the fundamental tests of hydrogenic and helium-like emission. The code's execution speed is affected by the number of coarse continuum cells due to the frequent reevaluations of the opacity and photo-interaction rates. For factors near unity the execution time will scale roughly inversely linearly.

The code can be sped up by making the factor larger than unity. But there is a limit, roughly 5, where the continuum cells become so coarse that the code will no longer pass its internal sanity checks. A factor near 2 will cut the execution time by about 40%. This will affect the predictions and should only be done in exploratory calculations.

set continuum shielding This changes the treatment of shielding of the incident continuum by line optical depths. There are several options. **`Pesc`** uses the inward-looking escape probability. **`Federman`** is the default and uses the function given in the appendix of Federman et al. (1979). **`Ferland`** uses the function given by Ferland (1992). **`None`** turns off self-shielding.

set fine continuum This changes the logic used to determine the resolution of the fine continuum mesh. The command has two arguments. The name of an element must appear on the line – the atomic weight of this element will be used to determine the narrowest lines that must be resolved. The number of resolution bins over a HWHM must also appear on the line.

16.16.9. set convergence …

The error in the heating-cooling balance is set with the **`set temperature convergence`** command (page 219 below). The error in the electron density is set with the **`set eden convergence`** command (page 211 below). The error in the local pressure is set with the **`set pressure convergence`** command (page 216 below). In cases where the code is having trouble converging the **`set presioniz`** command (page 215 below) will limit the number of ionization evaluations before declaring a failure.

16.16.10. set coverage [fast]

This limits the number of zones and iterations that will be done so that the code runs more quickly. It allows quick runs of the test suite with tools such as Purify and valgrind. If the **fast** option appears then only one and one iteration will be performed. Otherwise up to ten zones and two iterations will be done. This limit is imposed on top of whatever other limits may exist in the input stream.

16.16.11. set csupra = -12.34

This sets the secondary ionization rate due to supra-thermal electrons to the number on the line. The number is the log of the rate [s^{-1}]. The excitation rate of Lα is assumed to be the same. This option is used to test the code in secondary-ionization dominated cases. Normally the secondary ionization rate is determined self-consistently from the X-ray continuum or the **cosmic ray** command (see page 104 above).

16.16.12. set D/H -3.2

This sets the D/H abundance ratio. The default is the primordial abundance of 1.65×10^{-5} as measured by Pettini & Bowen (2001). The number is interpreted as the log of the D/H ratio if it is negative or the keyword **_log** appears, and as the linear ratio otherwise. This mainly affects HD cooling. Currently the molecular abundance ratio HD/H_2 is assumed to be equal to the D/H ratio.

16.16.13. set didz 0.05

The thickness of the first zone is chosen so that the largest continuous optical depth through it is one percent of the entered value. Thereafter the zone thickness is continuously adjusted by checking that the optical depth at the maximum continuum-gas interaction energy is set to this value. The default is 0.15. If the value is less than or equal to zero, then it is interpreted as the log of the quantity, and linear if greater than zero.

16.16.14. set _dr_ 11.2

This sets the zone thickness. There are spaces around the " **dr** ". The argument is the log of the thickness in cm and the default is 10^{31} cm. The number is interpreted as the linear thickness if the keyword **linear** appears.

16.16.15. set drmax 11.2

This sets the largest allowed zone thickness [cm]. The zone thickness will not become larger than this. The number is the log of the thickness if it is less than 38 or if the keyword **_log** appears. The default is 10^{31} cm.

16.16.16. set drmin 11.2

This sets the minimum zone thickness [cm]. The zone thickness will not become larger than this. The number is the log of the thickness if it is less than 38 or if the keyword **_log** appears. The default value is 10^{-20} cm.

16.16.17. set dynamics commands

These commands change aspects of dynamical or time-dependent calculations. They are described on page 117 above.

16.16.18. set eden [convergence, solver, value]

These commands affect the electron density or how it is determined.

set eden convergence 0.01 This sets the convergence criterion for the electron density. The number is the largest relative error in the electron density. It is interpreted as the log of the relative error if it is negative. The default value is 0.01. The old form of the command, **`set eden error`**, is also recognized.

set eden solver new This tells the code which solver to use to determine the electron density. There are currently two options, the default simple method, and a new method that is still under development. This command is currently under development and should not be used except under experimental conditions.

set eden 2.3 If no other keywords are recognized then this command sets the electron density. The number is the log of the density [cm^{-3}].

Note: The **`eden`** command (page 198 above) sets an extra source of electrons. This command sets the electron density itself. Both commands violate charge conservation.

16.16.19. set flxfnt -20

The highest photon energy that must be considered is lower for relatively soft continua such as a star than for X-ray sources such as AGNs. The criterion used to choose the highest energy to be considered ν_{high} is that $\nu f_\nu\,(\nu_{high})\ /\ \nu f_\nu\,(\nu_{peak}) <$ ***flxfnt***, where ν_{peak} is the frequency where the continuum reaches its maximum νf_ν. ***FluxFaint*** is normally 10^{-10}. This command changes the value of ***FluxFaint***. The argument is the log of the value.

16.16.20. set H2 ...

This command changes some aspects of the H_2 molecule. Other aspects of this molecule are changed with the **`atom H2`** command, described on page 85 above.

set H2 fraction This sets the ratio $n(H_2)/n(H)$. The number is interpreted as the log of the ratio if it is less then or equal to zero and as the linear ratio otherwise. An upper limit of 0.5 will be silently imposed. This command turns off the normal H_2 molecular network and forces the H_2 density to the hydrogen density multiplied by this fraction. This is totally unphysical and is only intended to provide an easy way to test the H_2 molecule.

set H2 Jura [TH85; CT02; SN99] This changes the “Jura rate”, the rate H_2 forms on grains. The default is the Cazaux & Tielens (2002) rate, which depends on grain temperature and abundance, and this can also be specified with the **`CT02`** option. The option **`TH85`** will use rates from Tielens & Hollenbach (1985a), and **`SN99`** will use rates for Sternberg & Neufeld (1999).

set H2 Jura scale The number on the line is a scale factor that multiplies the formation rate obtained by one of the above methods. If the scale factor is negative or the keyword **_log** appears then the number is interpreted as the log of the scale factor. Habart et al. (2003) suggest that the rate can vary across the galaxy by large factors.

set H2 Jura rate The number on the line is the log of the H_2 grain formation rate k [cm^3 s^{-1}]. This is used to give a simple grain formation rate $R = k\,n\left(\mathrm{H}_{tot}\right)n\left(\mathrm{H}^0\right)$ [cm^{-3} s^{-1}]. If no number appears on the line then the Jura (1975) rate of 3 × 10^{-17} will be assumed.

set H2 Solomon [BD96; TH85; ELWERT] This changes how the Solomon process is treated when the small H_2 molecule is used. The fits to the dissociation rate derived by Elwert et al. (2006) are the default and will be used if the keyword **ELWERT** appears. The keyword **BD96** will use Bertoldi & Draine (1996) and the keyword **TH85** will use the Tielens & Hollenbach (1985a) rate. These rates differ by ≥1 dex for some H_2 column densities. When the large H_2 molecule is used (see the **atom H2** command described on page 85 above) the Solomon process is treated in a self-consistent manner. Abel et al. (2004) show that H_2 column densities are quite sensitive to the correct treatment of this physics.

set H2 grain formation pumping This changes the distribution function for populations of v, J levels of H_2. There are three possible distributions: Takahashi (2001; **taka**); Draine & Bertoldi 1996; **DB96**); and thermal (**Thermal**).

set H2 Tad 420 This changes the binding energy, T_{ad}, in the formalism described by Le Bourlot (2000) to account for deexcitation of H_2 while on a grain surface. The number is the binding energy expressed as a temperature. The default value of 800 K maximizes the rates of H_2 collisional deexcitation and ortho-para conversion. If the number is ≤ 10 it is interpreted as a log of the temperature unless the keyword **linear** appears.

16.16.21. set HCORR

The density used in electronic collisions is actually $n_e + 1.7\times10^{-4}\,n\left(\mathrm{H}^0\right) f$. The second term is an approximate correction for collisions by neutral hydrogen. This is only a guestamite based on (Drawin 1969, see also Weisheit 1975, Steenbock & Holweger 1984, Lambert 1993, and Kiselman 2000). The number on this command adjusts the scale factor f. You can turn off the process by setting the number to zero.

16.16.22. set HO charge transfer [chemistry; ionization]

This changes the treatment of hydrogen – oxygen charge transfer. Charge transfer rates between atoms and the first ion of H and O are very fast and strongly couples their ionization (AGN3 Section 2.7). The process is normally treated as part of the chemistry network. The **ionization** option will include the rates within the ionization network instead. The chemistry and ionization solvers communicate and the result should not depend on which way the process is included. The strongly disturbed "Leiden hack" PDR models in the test suite require the **ionization** option to function properly.

16.16.23. set ind2 [_on_, _off]

This provides a way to turn off the affects of induced two-photon emission or absorption. One of the keywords **`_on_`** or **`_off`** must appear to turn induced two-photon processes on or off. It is on by default.

16.16.24. set kshell energy 1,000,000

This changes the energy of the highest continuum point considered for photoelectric opacity. The default is 1 MeV, sufficiently high that Compton recoil and pair production are the dominant opacity sources, and K-shell opacity may safely be ignored. Setting this limit to smaller values will save some compute time since the evaluation of the photoionization rate integrals will not extend to as high an energy. The argument is the energy in Rydbergs, and it must be greater than 194 Ryd. If zero is entered then the high-energy limit of the continuum will be used.

16.16.25. set Leiden hack

This replaces certain physical processes with the simple prescriptions that were specified for the 2004 Leiden PDR workshop (Röllig et al. 2007). These are only intended for testing and would not be used in a real calculation. If any **`set Leiden hack`** commands are entered the code will complain that a physical process has been disabled. This enables all hacks. Individual hacks can be turned on with additional keywords. They are:

set Leiden hack H2* off The chemistry network used in the workshop did not include H_2* (see Tielens & Hollenbach 1985a for a definition). This turns off reactions between that species and the CO network (although it is still present in the H-H_2 network).

set Leiden hack CR off. This turns off cosmic-ray excitation for the large H_2 molecule.

set Leiden hack UMIST This forces the code to use parts of the UMIST database that we feel that we do better with other methods.

16.16.26. set line precision [4, 5, or 6]

This changes how the emission lines are printed in the final pages of output. Emission-line wavelengths are normally printed with four digits, as in "4861". This command can increase the number of digits to 5 or 6. The lines are printed in four columns when four digits are chosen. With five or six digits the lines will no longer fit across the page so the number of columns is automatically reduced to three.

16.16.27. set nchrg 3

The grain physics uses an *n*-charge state model where, for each bin, the charge distribution is resolved in exactly *n* charge states, independent of grain size. This is discussed in van Hoof et al. (2004). The default value of *n* is 2 but can be reset with this command to any value between 2 and 5. Higher values of *n* will give more accurate results at the expense of greater compute time.

16.16.28. set negopc

Negative opacities may occur during a calculation if a level happens to mase (Ferland 1993). The code will generate a comment at the end if this happens. This command tells the code to punch the optical depth array when negative opacities occur. The output will go to the file ***negopc.txt***.

16.16.29. set nend 500

This sets the default limit to the number of zones that will be computed. The preset default limiting number of zones is 1400 but more zones may be needed in large column density clouds or ones exposed to very intense radiation fields.

The limit to the number of zones that will be computed can be set with either this command or with the **`stop zone`** command (page 127 above). The only difference is in the level of warning that will be generated if the code stops after reaching the limiting number of zones. If the code stops because it reached the number of zones set by the **`stop zone`** command then it thinks that this was the intended stopping criterion and no comment is generated. However the code generates a ***warning*** if it stops because it reaches the default limit to the number of zones since this probably *was not* intended. By using this command the limit can be increased while still retaining the checking and warnings that are generated if the code stops for an unintended reason.

The code allocates memory to store a great deal of information for each zone. Increasing the number of zones will also increase the memory needed to run the code.

16.16.30. set nFnu [options]

The continuum emitted by the central object and transmitted through the cloud, and the diffuse continuum produced by the cloud, will be printed within the emission-line printout if the command **`print continuum`** (page 132 above) is entered. The diffuse continua will be printed with the label *nFnu* and the transmitted incident continua are printed with the label *nInu*.

The **`set nFnu`** command changes which continua are included in the entry with the *nFnu* label. There are four possible continua, the transmitted and reflected incident continuum, and the transmitted and reflected diffuse continuum. Any or all of these may be entered, but at least one must occur. All four continua are included when the **`set nFnu`** command is parsed. Any component left off the command will not be included.

If this command is entered then **`print continuum`** does not also need to be given – the continuum points will occur in the printout. This command does not change the quantities printed with the *nInu* label – these are always the sum of the reflected plus transmitted incident continuum.

The four keywords, and the component that is included, are the following:

incident reflected or ***incident_reflected*** includes the incident reflected continuum.

incident transmitted or ***incident_transmitted*** includes the incident transmitted continuum.

diffuse inward or ***diffuse_inward*** includes the diffuse inward continuum.

diffuse outward or ***diffuse_outward*** includes the diffuse outward continuum.

All continua must be specified on the same **set** command. The following shows how to only include the outward incident and outward diffuse emission in the *nFnu* entry in the printout:

```
set nFnu diffuse outward, incident transmitted
```

16.16.31. set nmaps 50

This controls the number of steps in the heating-cooling map that results from either the **map** or **punch map** commands. Normally about 20 steps are taken between the lowest and highest temperatures.

16.16.32. set numerical derivatives

This tells the code to use numerical rather than analytic derivatives of the heating and cooling functions. The default is to use the analytic derivatives.

16.16.33. set PAH option

set PAH constant or H0 This changes the function that describes how PAH abundances depend on physical conditions. The default, which can also be specified with the keyword **H0**, is for the PAH abundance to scale as $n(H^0) / n(H_{tot})$. The abundance will be constant if the keyword **CONstant** appears. This is not physical and is only for testing.

set PAH BAKEs will replace our self-consistent treatment of PAH charging and heating with the heating equation given by Bakes & Tielens (1994). This is only intended for testing.

16.16.34. set path ="/usr/home/cloudy"

This command was removed in C07. You set the path by editing the file *path.cpp*. or by setting the environment variable *CLOUDY_DATA_PATH*.

16.16.35. set phfit [1995, 1996]

The key **1995** tells the code to use photoionization cross sections from Verner & Yakovlev (1995). The key **1996** is the default and uses Verner et al. (1996), which is partially based on Opacity Project cross sections.

16.16.36. set presioniz 50

This sets a limit to the number of times the bottom ionization solver will be called from the top pressure solver within a zone. This is a debugging aid and is only needed to shorten the number of convergence attempts within a zone that is destined to have a convergence failure.

16.16.37. set pressure convergence 0.01

This sets the convergence criterion for the total pressure. The number is the largest relative error in the pressure. The number is interpreted as the linear error if it is positive and the log of this error if negative. The default value is 0.01.

16.16.38. set punch commands

Punch output, described in the section beginning on page 138 above, is the primary output mechanism for the code. This command sets various details about how this output is generated.

set punch hash "newstring" When more than one iteration is punched into a file each ends with a series of hash marks that makes it easy to locate with an editor. This sets the hash string to something else. A new string must appear within the pair of double quotes.

The special string "**`return`**" is replaced with a single carriage return which translates into the pair of carriage returns that ***gnuplot*** uses to separate plots. The special string "**`time`**" will give the elapsed time since the start of time-dependent calculations. In both cases the keyword must appear within the pair of double quotes.

The hash can be completely turned off with the **`no hash`** option on the punch command (see page 140 above).

set punch prefix "test" This adds a prefix to all filenames and so provides an easy way to change all file names at one time. The prefix is any string that appears between the pair of double quotes on the command line.

set punch LWidth 10,000 km/sec The observed contrast between emission lines and the continuum depends on the intrinsic line width and, for an unresolved line, the resolution of the spectrometer. Lines are included in the continuum produced by the **`punch continuum`** commands (see page 143 above). This command adjusts the contrast between the lines and continuum.

Lines and continua are stored separately throughout the code. They are combined only when the output from the **`punch continuum`** command is produced using the expression

$$\nu F_\nu(\text{total}) = \nu F_\nu(\text{continuum}) + \frac{c}{PunchLWidth} I(\text{line}) \qquad (79)$$

where c is the speed of light. Values are entered in km s^{-1} and the default is 1000 km s^{-1} km s^{-1}.

If no number appears on the line, but the keyword _**`c`**_ does, the speed of light will be used. Note the space before and after the 'c'.

The intensities of the emission lines in the punch files, defined by subtracting the intensity in the continuum from the sum of the line and continuum, will be correct if the line width is set equal to the speed of light. The lines will have too small a contrast in that case, however, unless the spectrometer has a resolving power of unity. If the line width is smaller than the speed of light then the line to continuum contrast will be greater but the summed intensity of the line plus continuum in the punch output will be greater than the actual radiated power.

The only effect of this command is to change the line to continuum contrast in output from all **`punch`** commands except for that produced by the **`punch transmitted continuum`** command. Turbulent velocities are set with the **`turbulence`** command.

16.16.39. *set recombination* keywords

One of the keywords **`dielectronic`** or **`radiative`** must appear. This changes the treatment of various details of the ionic recombination physics.

The **`set dielectronic recombination`** command modifies the treatment of the low- and high-temperature contributors to the total dielectronic recombination rate coefficient. The default condition is for guestamates of third row and forth row elements to be used, the high-temperature (Burgess) process to be suppressed at high densities, but low-temperature recombination to be 100% efficient at all densities.

set dielectronic recombination kludge [options] At present rate coefficients for dielectronic recombination through low-lying autoionizing states have not been computed for lower stages of ionization of most elements on the third row and higher. The **`kludge`** option modifies the treatment of the guesses of the missing dielectronic recombination coefficients.

The default is to use means of all existing DR rates for each ion stage to replace missing data for that stage. For instance, $Fe^+ \Rightarrow Fe^0$ does not have reliable DR rates. Its rate will be the mean DR rate for all first ions of all elements with published rates.

The command **`set dielectronic recombination kludge`** will use the means of the rate coefficients for the four lowest stages of ionization of C, N, and O. These are $3\pm2\times10^{-13}$, $3\pm2\times10^{-12}$, $1.5\pm0.5\times10^{-11}$, and $2.5\pm1.4\times10^{-11}$ $cm^3 s^{-1}$ (see Ali et al 1991) and were the default DR kludge rates in C06.02 and before. The uncertainty is indicated by the quoted uncertainty, which is the dispersion from the mean of the quoted atoms and ions. Kraemer et al. and Badnell et al. give rate coefficients used for heavier elements. These are used for those ions that have no rate coefficients because no better can be done at present.

These rate coefficients can be turned off, or the values changed by a scale factor, with the **`set dielectronic recombination kludge`** command. If a number is entered on the line then it is the scale factor to multiply all the above rate coefficients. If no number is entered then zero is assumed and the effect is turned off. If more than one number is entered then each is used as a scale factor for successive stages of ionization. If fewer than 4 numbers are entered, then the last entered scale factor is used for higher stages of ionization.

set dielectronic recombination kludge Badnell This **`kludge`** option is the default. It uses the means of existing calculations of the rate in place of both low- and high-temperature DR. These means are done as a function of charge before recombination and have the advantage that they are based on real calculations at the current temperature.

set dielectronic recombination Burgess [_on_, _off] Rate coefficients for recombination at high temperatures are dominated by the Burgess (1965) process, which occurs though a pseudo-continuum of autoionizing levels. This process may be suppressed at high densities (Burgess and Summers 1969, Davidson 1975). Fits to Davidson's results are used if **Burgess on** appears. The process is assumed to be 100% efficient if **Burgess off** appears. The default is for suppression to be included.

set dielectronic recombination Nussbaumer [_on_, _off] Rate coefficients for recombination at nebular temperatures (i.e., where *kT* is much smaller than the ionization potential of the species) are dominated by a few autoionizing levels lying just above the ionization threshold (Nussbaumer and Storey 1983). This process may be suppressed at high densities (Davidson 1975). Fits to Davidson's results are used if **Nussbaumer on** appears. The process is assumed to be 100% efficient if **Nussbaumer off** appears. The default is for collisional suppression *not* to affect this process.

set dielectronic recombination [Badnell; old] This changes which set of dielectronic recombination rate coefficients are used. The **Badnell on** option is the default and tells the code to use the rate coefficients calculated by Badnell et al. in a series of papers that appeared in A&A. These supersede the various approximations described above. The old approximations will be used if the **Badnell off** option appears.

The **print** option will output both RR and DR rates for all species then stop.

set dielectronic recombination noise 2.1 This adds a component of Gaussian random noise to the guesses of the dielectronic recombination rate coefficients. The number on the line is the dispersion. The resulting random number will multiply the rate coefficient. The seed for the random number generator is set when this command is parsed. As a result the same DR rates will be used throughout any single calculation but the noise multiplying the rate will change from run to run.

set radiative recombination [Badnell; old] This changes which set of radiative recombination rate coefficients are used. The **Badnell on** option is the default and tells the code to use the rate coefficients calculated by Badnell et al. in a series of papers that appeared in A&A. The old approximations will be used if the **Badnell off** option appears.

The **print** option will output both RR and DR rates for all species then stop.

16.16.40. set spectrum [options]

This modifies the behavior of the **punch spectrum** command (see page 171 above). A series of **set spectrum** commands can occur and these modify any **punch spectrum** commands that follow them. The following shows an example of changing the resolution and then producing a **contin.dat** file.

```
set spectrum resolving power 100
```

```
punch spectrum "contin.dat"
```

The following are the options now recognized by the **`set spectrum`** command.

set spectrum range 1 to 5 Ryd This sets the energy range of the continuum that is predicted. The default, when this is not used, is to produce the full continuum. The energies are given in Rydbergs and (for now) and other units are not recognized.

set spectrum revolving power 1000 This sets the resolving power of the continuum that is predicted. The default, when this is not given, is to use the native resolution of the code.

16.16.41. set temperature [floor, solver, convergence]

The **`constant temperature`** command (see page 103 above) is used to set the temperature. These commands change some details of the thermal solution.

set temperature floor This sets a lowest kinetic temperature to allow in a calculation. When the temperature falls below this floor the code goes over to a constant temperature solution at the floor temperature. This provides a way to mimic having a minimum temperature that is set by some external and unspecified source of heat.

set temperature solver This tells the code which solver to use for the heating – cooling solution. The options are **`brent`** and **`simple`**. (**`brent`** is currently under development and should be used only for testing).

set temperature convergence The kinetic temperature is set by the balance between the heating and cooling. This command sets the relative error allowed in the heating-cooling match. The number is the largest fractional error allowed. It is interpreted as the error itself if it is positive and the log of the error if it is less than or equal to zero. The default is 0.005. This will be the error allowed in each zone. The total error or energy conservation mismatch integrated over a cloud will be much smaller, usually of order ten times smaller than the tolerance specified.

16.16.42. set test

This sets the logical variable ***lgTestCodeEnabled*** to true. It provides the facility to conditionally run test code somewhere in the main body of Cloudy.

16.16.43. set trimming –9 [upper lower, off]

The code saves execution time by not computing the population of stages of ionization with trivial abundances. The thresholds for excluding an ionization stage are chosen with photoionization equilibrium in mind. These may not be appropriate for some other conditions or if your definition of trivial is different from mine.

This command changes the limit for the smallest fractional abundance, $n(\mathrm{A}^{+x})/n(\mathrm{A})$, to consider. The smallest relative abundance to be considered for a stage of ionization higher than the ionization peak is changed with the **`upper`** keyword. The command **`set trimming upper off`** will turn off trimming of the highest stage of ionization. The smallest relative abundance of ions below the peak is changed with the **`lower`** keyword. The default relative ionization fractions are 10^{-6} and 10^{-10} respectively. If no keyword appears then both are changed to the number entered. The argument is the log of the lowest or highest ionization fraction to consider.

Generally, line excitation energies for atoms with stages of ionization higher than the peak ionization will strongly exceed the ambient temperature so these ions will have little influence on the calculated temperature or spectrum. This is not true for lines formed by ions below the peak distribution. The keyword **`off`** sets the smallest abundance to just above the machine's floating precision limit.

16.16.44. set tsqden 8

The code performs an analysis of the predicted emission-line spectrum at the end of the calculation. This analysis will find the structural t^2 as well as a t^2 deduced from the [O III] and H I spectrum (Kingdon & Ferland 1995 discuss this at length). Such an analysis only makes sense for densities below the critical density of the [O III] atom, which is $\sim 10^5$ cm^{-3}. The results of this analysis will not be printed if the density is higher than the value of ***tsqden***, currently 10^7 cm^{-3}. The number on the line is the log of the highest hydrogen density for which this analysis will be performed.

16.16.45. set UTA

This changes which UTA line data are used. Three sets of UTA data are available for some stages of ionization of iron. These include Behar et al. (2001), Gu et al. (2006; these papers consider Fe^0 through Fe^{+15}) and Kisielius et al. (2003; this includes Fe^{+13} though Fe^{+15} but has many more lines). Additional inner shell data are given by Behar & Netzer (2002). The Gu et al. (2006) results are used by default.

`set UTA Gu06 [on _off]` – this will enable or disable the Gu et al. (2006) rates. They are used by default.

`set UTA Kisielius [on _off]` – this will enable or disable the Kisielius et al. (2003) rates. They are disabled by default. The Behar or Gu data are replaced with the Kisielius et al. (2003) results for the three stages of ionization considered in that paper when this is enabled.

The **`no UTA`** command (page 205 above) turns off UTA ionization. .

16.16.46. set WeakHeatCool 0.02

This command sets the threshold for the weakest coolant or heat source included in output from the **`punch heating`** (page 155 above) or **`punch cooling`** (page 149 above) commands. The default is 0.05. The number entered is interpreted as a log if it is negative.

16.17. table lines "name.dat"

When the code is used as a subprogram for other, larger, codes, it is possible to read in a series of lines whose intensity will later be extracted by first calling ***cdGetLineList***, then by calling ***cdLine***. The procedure is described in Part 3 of this document. A set of lines that occur within any of several data files is then read. This method is used in most of the large grid programs I use.

This command provides a quick way to confirm that the list of lines in the line data files have valid names. The command takes the name of a file as its argument and checks that all lines can be found. See the discussion of ***cdGetLineList*** in Part 3 for further information.

16.18. test

This command does a "smoke test" and provides an easy way to do a quick sanity check on the code. It issues a series of commands to run a two-zone constant-temperature model. The **`table agn`** command is used with the density and temperature constant at 10^4. The ionization parameter is 10^{-2} and the calculation stops after two zones and one iteration. Many **`assert`** commands are used to verify predictions. The commands that set up the model will be printed if the keyword **`PRINT`** occurs on the line.

16.18.1. test FeII

When the **`FeII`** keyword appears the large Fe II atom (page 83 above) will be computed and checked as well.

16.18.2. test large

When the **`large`** keyword appears the model hydrogen atom (page 88 above) will be set to a large number of levels.

16.18.3. test H2

This tests the large H_2 molecule described on page 85 above.

16.18.4. test molecular

This does a simulation that is cold and nearly fully molecular. The can be combined with the **`H2`** keyword to test the H_2 molecule in the fully molecular limit.

16.19. Performance speedups

It is possible to speed up the calculation at the loss of some physical fidelity or stability. This section outlines the commands that make this possible. Each command is described in greater detail in sections earlier in this document.

Many of these options are included in the *fast.ini* initialization file. Using this *ini* file will decrease the execution time by roughly an order of magnitude. This is meant as a way to explore vast ranges of parameters or as a debugging aid.

N.B.!! The fidelity of the simulation is compromised! These turn off significant physical processes.

16.19.1. Turn off minor elements

The ionization distribution and the effects of an element on the gas cooling and opacity are all determined self-consistently. This includes the first 30 elements and many of these have trivial abundances. The calculation can be sped up with no loss of physical fidelity elements with very small abundances are turned off. This is done with the **`element off`** command described on page 55 above. The ini files *c84.ini,* *fast.ini*, and *ism.ini*, among others, include a set of **`element off`** commands to do this. The **`element limit`** command (page 56 above) provides a way to turn off all elements which have an abundance smaller than a specified limit.

Turning off an element will affect results if the opacity or cooling due to the element is significant. Minor elements can have major effects in very dense, optically thick, gas, where all coolants are close to the black body limit.

16.19.2. Turn off the chemistry

The chemical network requires a fair amount of time due to the size of the matrix that must be solved. The chemical state is determined even in ionized regions to ensure continuity in the transition between the H^+ – H^0 – H_2 regions. The chemistry can be safely ignored if only ionized regions are present. This is done with the **`no molecules`** command, described on page 203 above.

16.19.3. Turn off grain physics

The treatment of grain physics is today's state of the art (van Hoof et al. 2004) and can be CPU-intensive. Grains have several major effects. Elements locked up in solids are missing from the gas phase and so their cooling is also missing. Grains provide the dominant opacity across much of the optical, near IR, and UV spectrum. This absorbs the incident continuum, affects the radiative acceleration of the gas, and the transfer of optically thick lines. Radiative and collisional interactions between grains and the gas affect the gas temperature. In PDR and molecular regions, grains have an important effect on the charge balance of the gas. This affects both the ionization and chemistry (Abel et al. 2005). Grain surface reactions and molecular freeze-out change the chemistry and charge balance of the gas.

The first effect can be included at no expense by setting the gas-phase abundance of an element to a depleted value. Gas-phase abundances can be decreased by typical ISM depletion factors using the **`metals deplete`** command, described on page 66 above. This does not turn on grains and applying a depletion factor has no impact on the execution time.

Turn off quantum heating. Quantum heating is the process where a grain's temperature spikes after absorbing a single photon. This temperature spiking has an effect on the Wien tail of the grain's emitted spectral energy distribution but no other effect. Quantum heating can be disabled with the **`no qheat`** option on the **`grain`** command if the thermal continuum is not something you need to predict. Quantum heating only affects the emitted spectrum so turning if off will not affect results if the emitted IR continuum does not affect the gas. The IR continuum will affect the gas if it is absorbed by the gas or dust, which can occur with some line, or if the source is optically thick in the near IR continuum.

Use single rather than distributed grains. If the **`single`** keyword appears on the **`grain`** command then a single mean grain size will take be used instead of the size–resolved grain distribution. This affects the entire simulation, including the gas temperature and emission line spectrum, because the grain – gas interactions depend on the grain size.

Turning off all grain physics. All grain-gas interactions, except for their opacity, are turned off with the **`no grain physics`** command (page 202 above). Diffuse emission of the grains is no longer included so energy is not conserved. The dynamical and opacity effects of the grains will still be included.

grains no reevaluate. The **`no reevaluate`** option on the **`grains`** command will speed up a calculation by not reevaluating grain quantities all the time. Roughly a 30% speedup can be achieved. This is potentially dangerous and can destabilize a solution and/or lead to wrong results. It should be used under certain experimental circumstances, and not in a true simulation of a cloud.

16.19.4. Turn off line transfer

Many lines are optically thick. If the density is high then photons are thermalized after multiple scatterings. When dust opacities are present lines can also be absorbed by continuous absorption. In this case they act as an ionization and heating agent. The **`no line transfer`** command (page 203 above) turns off line transfer for all lines except the H and He Lα transitions. These assumptions are common in codes designed to treat classical nebulae but are not appropriate for dense gas.

16.19.5. Turn off level 2 lines

This is done with the **`no level2 lines`** command, described on page 203 above. The level 2 lines are a large set of transitions that came from the Opacity Project. They are important in dense or very high ionization gas. The Level 2 lines are important for pumping excited levels of many heavy elements. These include species such as CI*, CII*, etc.

16.19.6. Don't reevaluate the ionization or opacities

The **`no ionization reevaluate`** command (page 203 above) tells the code not to constantly reevaluate the level of ionization during the thermal solution. This may affect the code's stability for dense or dust-free gas but should not affect results.

The **`no opacity reevaluation`** command (page 204 above) tells the code not to reevaluate the opacities as it searches for a thermal solution. This may affect the code's stability for dense or dust-free gas but should not affect results.

These commands are safe when grains are present since their opacity strongly diminishes the diffuse radiation field. When grains are not present the diffuse radiation fields within the Balmer continuum or Lα can be quite intense and dominate the photoionization of some third row atoms. In this case constant reevaluation of the opacity and ionization is needed for a stable solution.

16.19.7. Turn off fine opacities.

The code uses a multi-grid approach to handle continuum interactions quickly, but also resolve lines so that line overlap can be treated in an automatic manner. There is a coarse continuum mesh, with a relatively low resolution and a high-resolution or fine mesh to resolve all lines. This second mesh is computationally expensive and is turned off with the **`no fine opacities`** command (page 202 above).

Turning off the fine mesh also turns off the treatment of line overlap and will affect results when overlap is important. There are many situations, like classical nebulae, where line overlap is not important.

16.19.8. Degrade the continuum resolution

The resolution of the coarse continuum mesh affects the execution time since photoionization rates and opacities involve repeated sums over it. The resolution is changed with the **`set continuum resolution`** command (page 209 above). This is not included in the *fast.ini* file since it is not possible to use the series of special incident continua that are part of the code distribution. It would be necessary to recompile these continua at the lower resolution (with the **`compile grains`**, page 193 and **`compile stars`** command, page 192 above) to use grains or stellar continua at lower resolution.

16.19.9. Make the iso-sequence model atoms as small as possible

The code treats several iso-sequences with a unified model atom. The execution time increases when the number of levels within the model atoms is increased. Less time will be used if the smallest possible number of levels is used. The number of levels is adjusted with the **`levels`** option on the **`atoms`** command, described on page 82 above. The **`atom levels`** commands for the H-like and He-like atoms accepts the keywords **`very small`** to make the atom as compact as possible. The line spectrum predicted by these atoms is likely to be highly inaccurate, and Case B intensities are far better when a compact model is used.

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