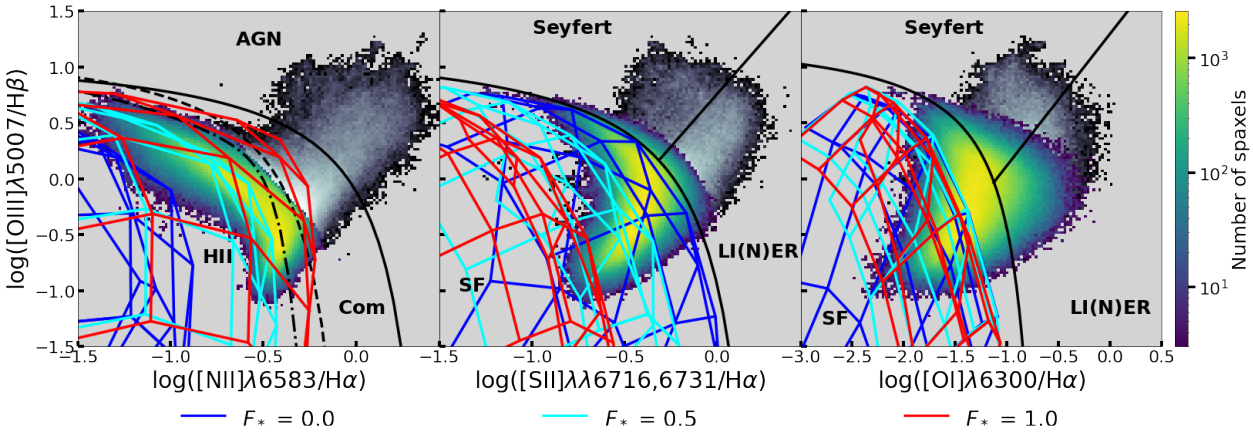

Hazy

a brief introduction to CLOUDY *C25*

2. Results, computational environment, and test suite

Cloudy & Associates

www.nublado.org

April 2, 2025

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Cover image: BPT diagrams showing effects of self-consistent grain depletions, from Gunasekera et al. (2023).

CONTENTS

LIST OF FIGURES ix

LIST OF TABLES xi

1 OUTPUT 1
- 1.1 Overview . . . 1
- 1.2 Header Information . . . 1
- 1.3 Chemical composition . . . 4
- 1.4 Comments before or during the calculation . . . 5
- 1.5 Zone Results . . . 5
- 1.6 Comments after the calculation . . . 9
- 1.7 Geometry . . . 12
- 1.8 Warnings, Cautions, Surprises, and Notes . . . 12
- 1.9 Optional Plot . . . 13
- 1.10 Final Printout . . . 14
  - 1.10.1 Intrinsic line intensities and luminosities . . . 15
  - 1.10.2 Emergent line intensities and luminosities . . . 15
  - 1.10.3 Air vs vacuum wavelengths . . . 16
  - 1.10.4 Some physical properties of the cloud . . . 16
  - 1.10.5 Average temperatures and densities . . . 19
  - 1.10.6 Average grain properties . . . 20
  - 1.10.7 Optical depths . . . 21
  - 1.10.8 Column densities . . . 22
  - 1.10.9 Mean ionization and temperature . . . 22
  - 1.10.10 Convergence statistics . . . 24
  - 1.10.11 Final report . . . 24

2 OBSERVED QUANTITIES 25
- 2.1 Overview . . . 25
- 2.2 Intensities of various continua . . . 25
  - 2.2.1 Incident radiation field . . . 25
  - 2.2.2 The radiation field at specific wavelengths . . . 25
  - 2.2.3 The radiation field integrated over a range of wavelengths . . . 25
- 2.3 Emission-Line Equivalent Widths . . . 26
- 2.4 Emission-Line Asymmetries . . . 27

2.5 Surface Brightness . . . 27
2.6 Flux to luminosity . . . 27
2.7 Flux at the Earth . . . 28
2.8 Relative hydrogen line intensities . . . 28
2.9 Helium line intensities . . . 28
2.10 Line intensities in a dusty cloud . . . 28
2.11 Continuum pumping contribution to line intensities . . . 31
2.12 Column densities . . . 31
2.13 A synthetic spectrum . . . 31
2.14 Line profiles . . . 32

3 LIMITS, ASSUMPTIONS, AND RELIABILITY 33
3.1 Overview . . . 33
3.2 Time steady . . . 33
3.3 Atomic and molecular database . . . 34
3.3.1 Collisional processes . . . 34
3.3.2 Photoionization cross sections . . . 35
3.3.3 Recombination rate coefficients . . . 35
3.3.4 Charge transfer . . . 35
3.4 Continuous opacity . . . 35
3.5 Temperature range . . . 36
3.6 Density range . . . 36
3.7 Radiative transfer . . . 37
3.8 Reliability . . . 37
3.9 The future . . . 38

4 THE CONTINUUM 39
4.1 Overview . . . 39
4.2 Attenuation of the incident continuum . . . 39
4.3 Recombination equilibrium . . . 39
4.3.1 On-the-spot approximation . . . 39
4.3.2 Outward only approximation . . . 40
4.4 Continuous opacities . . . 40
4.4.1 Total opacity arrays . . . 40
4.4.2 Cross-section array . . . 41
4.4.3 Photoionization rates . . . 41
4.4.4 Attenuation within the zone . . . 42
4.4.5 Rayleigh scattering . . . 42
4.4.6 Free-free opacity . . . 42
4.4.7 Bound-free opacity . . . 43
4.4.8 Plasma frequency . . . 44
4.4.9 Pressure lowering of ionization potential . . . 44
4.5 The frequency mesh . . . 44
4.5.1 Frequency mesh logic . . . 44
4.5.2 Routines defining the frequency mesh . . . 45

4.5.3 Changing the resolution of the mesh . . . 45
4.6 Continuum generation . . . 45
4.7 Energy units; the Rydberg . . . 46

5 LINE ATOMIC PARAMETERS 47
5.1 Overview . . . 47
5.2 Spectroscopic notation . . . 47
5.3 Line absorption . . . 48
5.3.1 Line optical depths . . . 48
5.3.2 Oscillator strengths . . . 48
5.3.3 Absorption cross section . . . 48
5.4 The line profile function . . . 49
5.4.1 Velocities in a thermal distribution . . . 49
5.4.2 Micro vs macro turbulence . . . 50
5.4.3 Line Widths . . . 50
5.4.4 The Doppler *b* parameter . . . 50
5.4.5 Voigt function . . . 51
5.4.6 Mean vs. line center optical depths . . . 51
5.5 The Einstein coefficients . . . 51
5.6 Continuum pumping . . . 52
5.6.1 Photon occupation number . . . 52
5.6.2 Pumping rates . . . 53
5.6.3 Optical depth effects . . . 53
5.7 Kirchhoff's Law . . . 55
5.8 The line source function and mean intensity . . . 55
5.9 Level populations in radiative equilibrium limit . . . 56

6 LINE DETAILS 57
6.1 Overview . . . 57
6.2 Line Boltzmann factors . . . 57
6.3 Air vs vacuum wavelengths . . . 57
6.4 The line escape probability functions . . . 58
6.4.1 Escape probability formalism vs exact radiative transfer . . . 58
6.4.2 Redistribution functions . . . 58
6.4.3 Incomplete redistribution . . . 58
6.4.4 Damping constant . . . 59
6.4.5 Background opacity and Destruction probability . . . 59
6.4.6 Complete redistribution . . . 59
6.4.7 Masing lines . . . 60
6.4.8 Stark broadening . . . 60
6.4.9 Net escape probability . . . 60
6.5 Optical depths and the geometry . . . 60
6.5.1 Open geometry . . . 61
6.5.2 Closed geometry overview . . . 61
6.5.3 Wind . . . 61

6.6 Collision strengths . . . 61
6.7 Born approximation . . . 62
6.8 The g-bar approximation . . . 62
6.9 The critical density . . . 63
6.10 Line thermalization length . . . 63
6.11 Averaging levels into terms . . . 63
6.11.1 Collision strengths . . . 63
6.11.2 Transition probabilities . . . 64
6.12 Level populations with collisions . . . 64

7 CLOUDY AS A STANDALONE PROGRAM 67
7.1 Running a single model with a shell script . . . 67
7.2 Running a single model from the command line . . . 68
7.3 Running grids of simulations or optimizing a simulation . . . 68
7.3.1 Grids of simulations . . . 69
7.3.2 Optimizing a simulation . . . 69
7.4 Parallel processing with MPI . . . 69

8 CLOUDY AS A SUBROUTINE 71
8.1 Overview . . . 71
8.1.1 Host languages . . . 71
8.1.2 Creating a new main program . . . 73
8.1.3 The cddefines.h and cddrive.h header files . . . 73
8.1.4 The template for main programs . . . 73
8.1.5 A note on return conditions . . . 74
8.2 Initializing the code . . . 74
8.3 Handling input and output . . . 74
8.3.1 cdTalk—produce output? . . . 74
8.3.2 cdOutput—sending output to a file . . . 74
8.3.3 cdInput—reading input from a file . . . 75
8.3.4 cdRead—entering Commands . . . 75
8.4 Executing the code . . . 76
8.4.1 cdDrive—calling the Code . . . 76
8.4.2 cdNoExec—checking without Computing . . . 76
8.5 Ending the code . . . 77
8.6 Checking Predictions . . . 77
8.6.1 cdB21cm—mean magnetic field . . . 77
8.6.2 cdColm—the computed column densities . . . 77
8.6.3 cdCooling_last—last zone's cooling . . . 78
8.6.4 cdDepth_depth—the depth structure of the cloud . . . 79
8.6.5 cdEDEN_last—electron density of last zone . . . 79
8.6.6 cdEmis—emissivity of lines . . . 79
8.6.7 cdGetLineList—sets of emission lines . . . 79
8.6.8 cdH2_colden—state-specific column densities of H_2 . . . 80
8.6.9 cdH2_Line—an H_2 emission line intensity . . . 80

8.6.10 cdHeating_last—last zone's heating . . . 81
8.6.11 cdIonFrac—the computed ionization fractions . . . 81
8.6.12 cdLine—emission-line intensities . . . 82
8.6.13 cdnZone—how many zones in the last iteration? . . . 83
8.6.14 cdPressure_depth—pressure structure of the last iteration . . . 83
8.6.15 cdPressure_last—pressure of the last zone . . . 84
8.6.16 cdTemp—the computed mean temperature . . . 84
8.6.17 cdTemp_last—the temperature of the last zone . . . 86
8.6.18 cdTimescales—several timescales. . . . 86
8.7 Other information . . . 86
8.7.1 cdDate(cdString) . . . 86
8.7.2 cdVersion(cdString) . . . 86
8.7.3 double cdExecTime() . . . 87
8.8 Printing comments . . . 87
8.8.1 Were comments generated? . . . 87
8.8.2 Printing the comments. . . . 87
8.8.3 cdErrors(FILE *io)—printing a summary of any problems . . . 88
8.8.4 cdPrintCommands(FILE *io)—print the command stack . . . 88
8.8.5 setbuf or the no buffering command . . . 88
8.9 Example Call as a Subroutine . . . 89
8.10 Computing Grids of Calculations . . . 90

9 THE EMISSION LINES 95
9.1 Overview . . . 95
9.2 The main emission-line printout . . . 95
9.2.1 Intrinsic and emergent line intensities . . . 95
9.2.2 Units of Line wavelengths . . . 95
9.2.3 Air vs vacuum wavelengths . . . 96
9.2.4 Blocks of lines in main output . . . 96
9.2.5 General properties. 96
9.2.6 Continua. 97
9.2.7 Molecules. 99
9.2.8 Species Bands. 99
9.2.9 Grains. 100
9.2.10 H-like iso-seq. 100
9.2.11 He iso-sequence. 102
9.2.12 Recombination. 102
9.2.13 Level 2 lines. 102
9.3 The transferred lines . . . 102
9.3.1 Save line data output . . . 102
9.3.2 Output produced for the transferred lines . . . 103
9.4 Line identifications . . . 104
9.5 Hydrogen recombination lines . . . 104
9.6 Molecular hydrogen lines . . . 104
9.7 CO lines . . . 105

10 PROBLEMS **109**
10.1 Introduction . . . 109
10.2 Thermal stability and temperature convergence . . . 109
10.2.1 Types of thermal maps . . . 109
10.2.2 No Temperature Convergence . . . 111
10.2.3 Thermal Stability . . . 113
10.2.4 Thermal fronts . . . 113
10.2.5 Map Output . . . 115
10.3 Convergence problems with dust-free static sphere . . . 116
10.4 Optical depth convergence problems . . . 116
10.5 Negative populations . . . 116
10.6 Floating Point Errors . . . 117
10.7 We can't fix it if we don't know it's broken . . . 117

11 HISTORY AND ACKNOWLEDGEMENTS **119**
11.1 History . . . 119
11.2 Acknowledgments . . . 119

A ATOMIC DATA SOURCES **123**

B GLOSSARY OF SYMBOLS **125**

C CONVERSION FACTORS **129**

D THE TEST SUITES **131**
D.1 Introduction . . . 131
D.2 Organization of commands . . . 131
D.3 The Auto Test Suite . . . 132
D.4 The Slow Test Suite . . . 390
D.5 Sample Programs . . . 414

REFERENCES **415**

LIST OF FIGURES

2.1 Dusty open geometry 30

4.1 free-free gaunt factors 43

5.1 Fluorescent pumping probability 54

8.1 C IV equivalent width 72

10.1 Cooling and heating in a photoionized gas 110
10.2 Cooling function for collisionally ionized gas 111
10.3 Temperature vs density in photoionization equilibrium 112
10.4 Thermal front example 114
10.5 Thermal front 114
10.6 Constant pressure thermal front 115

11.1 CLOUDY's size vs time 120

LIST OF TABLES

6.1 Line Boltzmann Factors 57

8.1 Special cases and examples, cdColm Column Densities 78

9.1 Default continuum bands 98
9.2 Hydrogen emission lines 104
9.3 Molecular hydrogen emission lines 106
9.4 CO emission lines 107

C.1 Conversion Factors 130

D.1 Keywords used in the Test Suite. 132
D.2 The simulations in the auto test suite. 132
D.2 (continued) 133
D.2 (continued) 134
D.2 (continued) 135
D.2 (continued) 136
D.2 (continued) 137
D.2 (continued) 138
D.2 (continued) 139
D.2 (continued) 140
D.3 The simulations in the slow test suite. 390

Chapter 1

OUTPUT

1.1 Overview

This section defines the output produced by CLOUDY. Each section begins with a sample of the output described, and then goes on to describe the meaning of the printout in greater detail. The output actually shown is from the Orion H II Region / PDR / molecular cloud test case (`orion_hii_pdr_pp.in`).

1.2 Header Information

Several lines of output echo the input commands and outline some properties of the initial continuum.

```
                                Cloudy 06.01.02

************************************06Jan02*************************************
*                                                                              *
* title the Orion HII Region / PDR / Molecular cloud with an open geometry     *
* #                                                                            *
* # commands controlling continuum =========                                   *
* # the incident continuum is two parts                                        *
* # kurucz continuum and flux of photons striking cloud                        *
* # this is the photosphere of the OVI star, its temperature and phi(H)        *
* table star kurucz 39600K                                                     *
* phi(H) 13                                                                    *
* # this adds the observed hot brems                                          *
* # its temperature (as log of T) and the flux of                             *
* # photons striking the cloud                                                *
* brems 6                                                                      *
* phi(h) 10                                                                    *
* #                                                                           *
* # cosmic rays are important for pdr chemistry                                *
* cosmic rays, background                                                      *
* #                                                                           *
* # commands controlling geometry  =========                                   *
* # this turns off the stop temperature option                                 *
* # so the sim will not stop due to temperature                                *
* stop temperature off                                                         *
* # this sets the thickness of the HII region & PDR                           *
* stop thickness 0.5 linear parsec                                             *
* # this will result in a milli gauss B-field in molecular region             *
* magnetic field -5 gauss                                                      *
* # assume constant pressure                                                  *
* constant pressure                                                            *
* set nend 2000                                                                *
* #                                                                           *
* # other commands for details     =========                                  *
* failures 3                                                                   *
* # mimic existence of unmodeled molecular gas                                 *
* double                                                                       *
* # iterate since lines optically thick                                       *
* iterate                                                                      *
* # set microturbulence in equipartition with B field                          *
```

```
* turbulence equipartition                                                    *
* # set the line width so lines appear on the save continuum                 *
* set SaveLwidth 10 km/s                                                     *
* #                                                                          *
* # commands for density & abundances =========                              *
* # this is the log of the initial H density, cm-3                          *
* hden 4                                                                     *
* # this will speed up the calculation a bit                                 *
* init file="ism.ini"                                                        *
* # this uses HII region abundances, but no grains                           *
* abundances hii region no grains                                            *
* # this uses orion grains                                                   *
* grains orion                                                               *
* >>>> mie_read_opc reading file -- graphite_orion_10.opc                <<<< *
* >>>> mie_read_opc reading file -- silicate_orion_10.opc                <<<< *
* # turn on PAHs, with an abundance that depends on H0 fraction,            *
* # as suggested by long-slit observations of Orion bar,                    *
* # with an abundance 3x larger than default built into the code            *
* grains pah function 3                                                      *
* >>>> mie_read_opc reading file -- pah1_bt94_10.opc                     <<<< *
* #                                                                          *
* # commands controlling output    =========                                *
* # print lots of faint CO lines                                             *
* print line faint -4                                                        *
* # normalize to Ha                                                          *
* normalize to "H  1" 6563                                                   *
* #                                                                          *
* # orion hii pdr pp.in                                                      *
* # class hii pdr                                                            *
*                                                                            *
******************************************************************************
```

This begins with the version number of CLOUDY, the date that the version was released, in the form yy.mm.dd. The following line gives this date in another form.

All of the input command lines, with the exception of those starting with a #, %, or *, are echoed before the calculation begins, and are saved to be reprinted after the calculation is completed.

```
3198CellPeak1.00E+00   Lo 9.99e-09=912.21cm   Hi-Con:1.20E+02 Ryd   E(hi):7.35E+06Ryd     E(hi):     100.01 MeV
I(nu>1ryd):   2.4792   Average nu:1.382E+00   I( X-ray):  -1.6194   I(BalC):   2.8255     Phi(BalmrC):  13.7081
phi(1.0-1.8):12.9508   phi(1.8-4.0): 12.033   phi(4.0-20):  9.388   phi(20--):  7.634     Ion pht flx:1.001E+13
I(gam ray):   0.0000   phi(gam r):   0.0000   I(Infred):   1.5064   Alf(ox):   0.0000     Total inten:   3.0012
U(1.0----):3.339E-02   U(4.0----):8.293E-06   T(En-Den):4.586E+01   T(Comp):3.532E+04     nuJnu(912A):5.422E+02
Occ(FarIR):2.911E+08   Occ(H n=6):1.326E-11   Occ(1Ryd):2.470E-14   Occ(4R):5.400E-20     Occ (Nu-hi):1.201E-32
Tbr(FarIR):4.835E+05   Tbr(H n=6):5.816E-08   Tbr(1Ryd):3.905E-09   Tbr(4R):3.413E-14     Tbr (Nu-hi):2.269E-25
```

This block of information describes the continuum that strikes the illuminated face of the cloud. The full block of information is shown above, and in the following discussion each line is given again just before it is described.

```
3198CellPeak1.00E+00   Lo 9.99e-09=912.21cm   Hi-Con:1.20E+02 Ryd   E(hi):7.35E+06Ryd     E(hi):     100.01 MeV
```

This gives the number of numerical frequency cells in the continuum followed by the energy (in Ryd) of the peak of hydrogen-ionizing continuum. This is the point with the largest flux density per unit energy interval (J_ν). Next is the energy of the low-energy limit of the continuum, in both Ryd and cm. The last two numbers are the energies of the high-energy limit of the continuum in Ryd and MeV.

```
I(nu>1ryd):   2.4792   Average nu:1.382E+00   I( X-ray):  -1.6194   I(BalC):   2.8255     Phi(BalmrC):  13.7081
```

This line gives the intensity or luminosity of the continuum source. Luminosities are printed if the inner radius of the cloud is specified. The units will be energy radiated by the central object into 4π sr [erg s^{-1}]. If an inner radius is not set then the code will compute the intensity case and give the emission per unit area of cloud surface. This is loosely called the intensity but is more formally $4\pi J$ where J is the proper mean intensity [erg cm^{-2} s^{-1} sr^{-1} for an emission line; AGN3 Appendix 1].

The line gives the log of the energy (erg s^{-1} cm^{-2} or erg s^{-1}, depending on whether it is the intensity or luminosity case) in the hydrogen-ionizing continuum (1 Ryd $\leq h\nu <$ 100 MeV), and

the average energy of the hydrogen-ionizing continuum, in Ryd, weighted by photon number;

$$\langle h\nu \rangle = \frac{\int_{1\,Ryd}^{\infty} 4\pi\, J_\nu\, d\nu}{\int_{1\,Ryd}^{\infty} 4\pi\, J_\nu / h\nu\, d\nu} \quad [\mathrm{Ryd}]. \tag{1.1}$$

The log of the energy in the X-ray continuum (20.6 Ryd $\leq h\nu \leq$ 7676 Ryd) is followed by the log of the energy (erg s^{-1} cm^{-2} or erg s^{-1}) and the number of photons (cm^{-2} s^{-1} or s^{-1}) in the Balmer continuum (0.25 Ryd to 1.0 Ryd).

```
phi(1.0-1.8):12.9508   phi(1.8-4.0): 12.033   phi(4.0-20):  9.388   phi(20--):  7.634     Ion pht flx:1.001E+13
```

The third line gives the log of the number of photons (cm^{-2} s^{-1} or s^{-1}) in four frequency bins (1.0 Ryd $\leq h\nu <$ 1.807 Ryd, 1.807 Ryd $\leq h\nu <$ 4.0 Ryd, 4.0 Ryd $\leq h\nu <$ 20.6 Ryd, and 20.6 Ryd $\leq h\nu <$ 7676 Ryd). The last number "Ion pht flx" is the flux of hydrogen ionizing photons;

$$\Phi\left(\mathrm{H}^0\right) = \frac{Q\left(\mathrm{H}^0\right)}{4\pi r^2} \quad [\mathrm{cm}^{-2}\mathrm{s}^{-1}]. \tag{1.2}$$

In this equation $Q(\mathrm{H}^0)$ is the total number of hydrogen-ionizing photons emitted by the central object (s^{-1}), and r is the separation between the center of the central object and the illuminated face of the cloud. Unlike the majority of the quantities printed in the header, $\Phi(\mathrm{H}^0)$ (per unit area) is always printed, never $Q(\mathrm{H}^0)$ (into 4π sr).

```
I(gam ray):   0.0000   phi(gam r):   0.0000   I(Infred):   1.5064   Alf(ox):   0.0000     Total inten:   3.0012
```

The fourth line of the header gives some information about the low and high energy portions of the incident continuum. The first number is the log of the luminosity or intensity in the gamma-ray ($\sim$100 keV to $\sim$100 MeV) continuum. The second number is the log of the number of photons over this energy range. The third number is the log of the luminosity in the continuum between 0.25 Ryd and the lowest energy considered, presently an energy of 3.040×10^{-9} Ryd. All of these entries are either per unit area, or radiated into 4π sr, depending on whether the intensity or luminosity case was specified.

The entry "Alf(ox)" is the spectral index α_{ox}, defined as in Zamorani et al. (1981), except for the difference in sign convention. This 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,

$$\frac{f_\nu\,(2\,\mathrm{keV})}{f_\nu\left(2500\,\mathrm{\AA}\right)} = \left(\frac{\nu_{2\,\mathrm{keV}}}{\nu_{2500\,\mathrm{\AA}}}\right)^{\alpha} = 403.3^{\alpha}. \tag{1.3}$$

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 $\alpha_{ox} \sim -1.4$. If no X-rays are present then $\alpha_{ox} = 0$. The last number on the line is the log of the total energy in the continuum between 3.040×10^{-9} Ryd and 100 MeV.

```
log L/Lsun:   3.9743   Abs bol mg:  -5.1858   Abs V mag:   2.4170   Bol cor:  -7.6028     nuFnu(Bbet):  34.5867
```

This line is optional, depending on whether the luminosity or intensity case is specified. (It was not printed in this model since we are working in the intensity case but a sample is shown). This is printed in the luminosity case. First comes the log of the total luminosity in the continuum in solar units. The absolute bolometric magnitude, absolute V magnitude, and the bolometric correction, are then given, followed by the log of the continuum specific luminosity $[\nu F_\nu(\mathrm{H}\beta)]$ at the wavelength of Hβ [erg s^{-1}].

```
U(1.0----):3.339E-02   U(4.0----):8.293E-06   T(En-Den):4.586E+01   T(Comp):3.532E+04     nuJnu(912A):5.422E+02
```

This line begins with two ionization parameters. The first is the dimensionless ratio of ionizing photon to hydrogen densities, defined as

$$U \equiv \frac{\Phi\left(\mathrm{H}^0\right)}{n_{\mathrm{H}} c}, \tag{1.4}$$

where n_H is the total hydrogen density. The second number is defined in a similar way, but the numerator is the number of photons with energies greater than 4 Ryd (i.e., helium-ionizing). The third number is the equivalent black-body temperature corresponding to the energy density u at the illuminated face of the cloud, from the incident continuum and Stefan's radiation density constant a;

$$T_u \equiv \left(L/4\pi r^2 ac\right)^{1/4} \quad [\mathrm{K}]. \tag{1.5}$$

T(Comp) is the Compton temperature of the incident radiation field.[1] The last number is $4\pi\nu J_\nu(912\text{Å})$, the flux at 912Å (erg cm^{-2} s^{-1}), where J_ν is the mean intensity of the incident continuum (Mihalas, 1978).

```
Occ(FarIR):2.911E+08   Occ(H n=6):1.326E-11   Occ(1Ryd):2.470E-14   Occ(4R):5.400E-20     Occ (Nu-hi):1.201E-32
Tbr(FarIR):4.835E+05   Tbr(H n=6):5.816E-08   Tbr(1Ryd):3.905E-09   Tbr(4R):3.413E-14     Tbr (Nu-hi):2.269E-25
```

These lines give dimensionless photon occupation numbers $\eta(\nu)$, for the incident continuum at several energies. The occupation number is defined as

$$\eta_\nu \equiv J_\nu(\nu)\left(\frac{2h\nu^3}{c^2}\right)^{-1}, \tag{1.6}$$

and the incident continuum brightness temperature $T_b(\nu)$, [K] is defined as

$$T_b(\nu) \equiv J_\nu(\nu)\left(\frac{2k\nu^2}{c^2}\right)^{-1} \quad [\mathrm{K}]. \tag{1.7}$$

These energies correspond to the lowest frequency considered (presently 10 MHz); the ionization potential of the $n = 6$ level of hydrogen (1/36 Ryd); one Rydberg; four Rydbergs, and the high-energy limit of the incident continuum. The energy where the last number is evaluated depends on the continuum shape. The energy is given by the fifth number on the first line of the continuum output.

1.3 Chemical composition

```
                                    Gas Phase Chemical Composition
H :  0.0000  He: -1.0159  Li: -9.4456  Be:-10.7418  B :-10.0360  C : -3.9385  N : -4.1002  O : -3.4622  F : -7.9927
Ne: -4.0501  Na: -6.3298  Mg: -5.0788  Al: -7.4597  Si: -5.9133  P : -7.0617  S : -4.7399  Cl: -7.0675  Ar: -5.3799
K : -7.3439  Ca: -9.5901  Sc:-11.1518  Ti: -9.0969  V :-10.1537  Cr: -8.5017  Mn: -7.7212  Fe: -6.4597  Co: -9.0200
                                       Ni: -7.7100  Cu: -8.6596  Zn: -7.9022
```

[1] For a blackbody radiation field $T_{Compton}$ is roughly 4% lower than the blackbody color temperature T_{color} when the energy density temperature T_u is $> T_{color}$. Only when $T_u \equiv T_{color}$ does induced Compton heating cause $T_{Compton} \equiv T_{color}$. If $T_u > T_{color}$ then $T_{Compton} > T_{color}$ because of induced Compton heating. All of the relevant physics is included in the Compton temperature printed here.

```
                    Grain Chemical Composition
C : -3.5553  O : -3.8821  Mg: -4.4841  Si: -4.4841  Fe: -4.4841
                  Sum Atoms Depleted: -3.2828
                  Depletion/Grains-1: 2.65%

                 Number of grains per hydrogen
Carbonaceous: -14.166  silicate: -14.103
```

The chemical composition of the cloud comes next. The three blocks of numbers give the gas-phase abundances of the elements, the abundances contained in grains, and the number of each type of grains per unit hydrogen. The numbers are the logs of the number densities of the elements, relative to the gas-phase hydrogen abundance of unity (so, 0 on the log scale). The sum of all atoms depleted with the **metals deplete** command is given in `Sum Atoms Depleted`. This is not guaranteed to agree with the atoms depleted with **grains** command. The percent offset is reported in `Depletion/Grains-1`. Only the active elements are included (those turned off with the **elements off** command are not printed). If grains are not present then the second two blocks are not printed.

1.4 Comments before or during the calculation

The code may print comments as the calculation proceeds. These are printed with the start of the comment in capital letters to make them easy to find with a script. The comments fall into three categories:

DISASTER something has unexpectedly caused the calculation to stop. The results are bogus and should not be trusted. The code should immediately return to the calling program.

PROBLEM something did not go as expected but the calculation is continuing. This might be a convergence failure at a point in the cloud. This is an indication that the code was having difficulties and a few of these can occur in a normal set of calculations. The predictions can be used if only a few occur and if the comments at the end of the calculation (see page 9 below) do not identify other problems.

NOTE this gives advice about the calculation. These can be ignored if you prefer.

1.5 Zone Results

Next comes a summary of the conditions in the first and last zone. This print out is done in routine *PrtZone* which should be consulted if there are any questions. The following is the output produced for one zone. Details follow.

```
####  1  Te:9.361E+03 Hden:1.000E+04 Ne:1.101E+04 R:1.000E+30 R-R0:5.223E+11 dR:1.045E+12 NTR:  3 Htot:3.461E-16 T912: 1.48e-05###
 Hydrogen      2.15e-04 1.00e+00 H+o/Hden 1.00e+00 1.00e-11 H-    H2 5.27e-19 3.99e-13 H2+ HeH+ 2.03e-14 Ho+ ColD 2.38e+14 1.11e+18
 Deuterium     2.15e-04 1.00e+00 D+o/Dden 1.00e+00 5.61e-12 D-    HD 6.70e-16 2.92e-12 HD+ HeD+ 1.40e-14 Do+ ColD 3.93e+09 1.83e+13
 Helium        6.57e-04 9.45e-01 5.47e-02 He I2SP3 3.52e-06 Comp H,C 1.75e-22 4.64e-23 Fill Fac 1.00e+00 Gam1/tot 1.00e+00
 He singlet n  6.54e-04 2.35e-11 6.59e-18 2.09e-18 3.18e-18 2.52e-18 He tripl 3.52e-06 9.32e-16 7.41e-18 4.77e-17 7.56e-18
 Pressure      NgasTgas 2.06e+08 P(total) 2.84e-08 P( gas ) 2.84e-08 P(Radtn) 1.79e-11 Rad accl 3.51e-05 ForceMul 3.33e+03
               Texc(La) 4.21e+03 T(contn) 4.59e+01 T(diffs) 2.03e+00 nT (c+d) 1.16e+07 Prad/Gas 6.30e-04 Pmag/Gas 2.80e-04
 gra-orion01*  DustTemp 2.12e+02 Pot Volt 5.32e+00 Chrg (e) 1.21e+02 drf cm/s 4.83e+03 Heating: 4.26e-18 Frac tot 1.23e-02
 gra-orion02*  DustTemp 2.02e+02 Pot Volt 5.08e+00 Chrg (e) 1.43e+02 drf cm/s 5.26e+03 Heating: 3.69e-18 Frac tot 1.07e-02
 gra-orion03*  DustTemp 1.91e+02 Pot Volt 4.86e+00 Chrg (e) 1.70e+02 drf cm/s 5.60e+03 Heating: 3.21e-18 Frac tot 9.26e-03
 gra-orion04*  DustTemp 1.81e+02 Pot Volt 4.66e+00 Chrg (e) 2.01e+02 drf cm/s 5.86e+03 Heating: 2.79e-18 Frac tot 8.06e-03
 gra-orion05   DustTemp 1.70e+02 Pot Volt 4.47e+00 Chrg (e) 2.39e+02 drf cm/s 6.07e+03 Heating: 2.43e-18 Frac tot 7.03e-03
 gra-orion06   DustTemp 1.60e+02 Pot Volt 4.30e+00 Chrg (e) 2.85e+02 drf cm/s 6.22e+03 Heating: 2.13e-18 Frac tot 6.16e-03
 gra-orion07   DustTemp 1.50e+02 Pot Volt 4.15e+00 Chrg (e) 3.40e+02 drf cm/s 6.33e+03 Heating: 1.87e-18 Frac tot 5.41e-03
 gra-orion08   DustTemp 1.40e+02 Pot Volt 4.02e+00 Chrg (e) 4.07e+02 drf cm/s 6.42e+03 Heating: 1.65e-18 Frac tot 4.77e-03
```

```
gra-orion09   DustTemp 1.31e+02 Pot Volt 3.91e+00 Chrg (e) 4.89e+02 drf cm/s 6.48e+03 Heating: 1.46e-18 Frac tot 4.21e-03
gra-orion10   DustTemp 1.22e+02 Pot Volt 3.80e+00 Chrg (e) 5.89e+02 drf cm/s 6.54e+03 Heating: 1.29e-18 Frac tot 3.73e-03
sil-orion01*  DustTemp 1.55e+02 Pot Volt 2.85e+00 Chrg (e) 6.44e+01 drf cm/s 1.45e+04 Heating: 2.44e-18 Frac tot 7.06e-03
sil-orion02*  DustTemp 1.49e+02 Pot Volt 2.70e+00 Chrg (e) 7.58e+01 drf cm/s 1.62e+04 Heating: 2.09e-18 Frac tot 6.03e-03
sil-orion03*  DustTemp 1.43e+02 Pot Volt 2.57e+00 Chrg (e) 8.92e+01 drf cm/s 1.77e+04 Heating: 1.78e-18 Frac tot 5.15e-03
sil-orion04   DustTemp 1.37e+02 Pot Volt 2.44e+00 Chrg (e) 1.05e+02 drf cm/s 1.91e+04 Heating: 1.53e-18 Frac tot 4.42e-03
sil-orion05   DustTemp 1.31e+02 Pot Volt 2.33e+00 Chrg (e) 1.24e+02 drf cm/s 2.02e+04 Heating: 1.32e-18 Frac tot 3.81e-03
sil-orion06   DustTemp 1.26e+02 Pot Volt 2.24e+00 Chrg (e) 1.47e+02 drf cm/s 2.11e+04 Heating: 1.14e-18 Frac tot 3.30e-03
sil-orion07   DustTemp 1.20e+02 Pot Volt 2.15e+00 Chrg (e) 1.76e+02 drf cm/s 2.18e+04 Heating: 9.93e-19 Frac tot 2.87e-03
sil-orion08   DustTemp 1.15e+02 Pot Volt 2.08e+00 Chrg (e) 2.10e+02 drf cm/s 2.23e+04 Heating: 8.67e-19 Frac tot 2.50e-03
sil-orion09   DustTemp 1.10e+02 Pot Volt 2.01e+00 Chrg (e) 2.52e+02 drf cm/s 2.26e+04 Heating: 7.60e-19 Frac tot 2.20e-03
sil-orion10   DustTemp 1.06e+02 Pot Volt 1.96e+00 Chrg (e) 3.03e+02 drf cm/s 2.28e+04 Heating: 6.69e-19 Frac tot 1.93e-03
pah-bt9401 *  DustTemp 3.41e+02 Pot Volt 6.60e+00 Chrg (e) 1.06e+00 drf cm/s 1.97e+02 Heating: 9.29e-22 Frac tot 2.68e-06
pah-bt9402 *  DustTemp 3.44e+02 Pot Volt 6.64e+00 Chrg (e) 1.28e+00 drf cm/s 2.13e+02 Heating: 1.01e-21 Frac tot 2.92e-06
pah-bt9403 *  DustTemp 3.47e+02 Pot Volt 6.61e+00 Chrg (e) 1.49e+00 drf cm/s 2.37e+02 Heating: 1.07e-21 Frac tot 3.08e-06
pah-bt9404 *  DustTemp 3.50e+02 Pot Volt 6.54e+00 Chrg (e) 1.70e+00 drf cm/s 2.67e+02 Heating: 1.09e-21 Frac tot 3.16e-06
pah-bt9405 *  DustTemp 3.53e+02 Pot Volt 6.44e+00 Chrg (e) 1.92e+00 drf cm/s 3.02e+02 Heating: 1.09e-21 Frac tot 3.16e-06
pah-bt9406 *  DustTemp 3.55e+02 Pot Volt 6.45e+00 Chrg (e) 2.22e+00 drf cm/s 3.29e+02 Heating: 1.13e-21 Frac tot 3.26e-06
pah-bt9407 *  DustTemp 3.57e+02 Pot Volt 6.47e+00 Chrg (e) 2.54e+00 drf cm/s 3.60e+02 Heating: 1.17e-21 Frac tot 3.38e-06
pah-bt9408 *  DustTemp 3.59e+02 Pot Volt 6.43e+00 Chrg (e) 2.87e+00 drf cm/s 4.00e+02 Heating: 1.18e-21 Frac tot 3.40e-06
pah-bt9409 *  DustTemp 3.61e+02 Pot Volt 6.46e+00 Chrg (e) 3.27e+00 drf cm/s 4.35e+02 Heating: 1.20e-21 Frac tot 3.46e-06
pah-bt9410 *  DustTemp 3.63e+02 Pot Volt 6.48e+00 Chrg (e) 3.71e+00 drf cm/s 4.74e+02 Heating: 1.22e-21 Frac tot 3.52e-06
Carbon        6.76e-07 1.91e-02 9.70e-01 1.10e-02 1.77e-04 2.36e-09 0.00e+00 H2O+/O   0.00e+00 OH+/Otot 0.00e+00 Hex(tot) 0.00e+00
Nitrogen      1.60e-06 1.72e-02 9.69e-01 1.41e-02 4.77e-05 1.34e-07 9.81e-14 0.00e+00 O2/Ototl 0.00e+00 O2+/Otot 0.00e+00
Oxygen        9.23e-06 1.17e-01 8.59e-01 2.47e-02 6.97e-05 9.60e-08 4.83e-11 0.00e+00 0.00e+00
Neon          5.77e-05 3.93e-01 5.95e-01 1.17e-02 7.25e-05 5.08e-08 1.99e-12 1.47e-16 0.00e+00 0.00e+00 0.00e+00
Magnesium     6.41e-06 7.31e-03 9.65e-01 2.74e-02 1.76e-04 5.41e-07 2.86e-10 3.72e-14 9.96e-19 0.00e+00 0.00e+00 0.00e+00 0.00e+00
Silicon    0  1.13e-07 8.39e-03 8.16e-01 1.56e-01 1.86e-02 4.68e-05 3.08e-08 5.13e-12 1.63e-16 0.00e+00 0.00e+00 0.00e+00 0.00e+00
Sulphur    0  7.25e-08 7.46e-03 9.03e-01 8.81e-02 1.60e-03 1.67e-04 5.91e-06 9.11e-10 3.49e-14 3.20e-19 0.00e+00 0.00e+00 0.00e+00
Chlorine   0  2.51e-07 1.32e-02 9.57e-01 2.92e-02 7.57e-04 5.50e-05 7.07e-07 9.54e-09 2.94e-13 2.17e-18 0.00e+00 0.00e+00 0.00e+00
Argon      0  9.50e-08 2.83e-03 9.69e-01 2.73e-02 4.35e-04 2.65e-05 3.24e-07 1.53e-09 1.16e-11 8.21e-17 0.00e+00 0.00e+00 0.00e+00
Iron       0  1.78e-08 2.88e-04 1.08e-01 8.56e-01 3.26e-02 2.33e-03 2.33e-05 2.30e-07 1.28e-10 1.94e-14 9.07e-19 0.00e+00 0.00e+00
```

The results of calculations for the first and last zones are always printed. Results for intermediate zones can be printed if desired (see the **print every** command). The following is a line-by-line description of the output produced for each printed zone.

```
####  1  Te:9.361E+03 Hden:1.000E+04 Ne:1.101E+04 R:1.000E+30 R-R0:5.223E+11 dR:1.045E+12 NTR:  3 Htot:3.461E-16 T912: 1.48e-05###
```

The line begins with a series of #### characters to make it easy to locate with an editor. The zone number is the first number and it is followed by the electron temperature of the zone ("Te"). A lower case "u" will appear before the "Te" if the temperature solution is possibly thermally unstable. This occurs when the derivative of the net cooling with respect to temperature is negative. This is discussed further in the section on thermal stability problems starting on page 109 below. The total hydrogen ("Hden") and electron ("Ne") densities (cm^{-3}) follow. The next number ("R") is the distance from the center of the central object to the center of the zone. The depth, the distance between the illuminated face of the cloud and the center of the zone, ("R-R0", or "r-r^o"), and the thickness of the zone ("dR", or δr), (all are in cm), follow. The inner edge of the zone is $(r - r_o) - \delta r/2$ from the illuminated face of the cloud. The line ends with a number indicating how many ionization iterations were needed for this zone to converge (NTR), followed by the total heating[2] ("Htot"; photoelectric and otherwise, erg cm^{-3} s^{-1}), and the optical depth between the *illuminated* face of the cloud and the *outer* edge of the zone at the Lyman limit (T912; the number is the *total absorption* optical depth at 912Å, and not the hydrogen Lyman-limit optical depth).

```
WIND; V:-7.000e+00km/s G:-0.00e+00 Accel: 8.62e-06 Fr(cont): 1.000 Fr(line): 0.000 Fr(dP): 0.000
```

A line describing the velocity and acceleration of the zone is printed if the cloud is a wind. The numbers are the wind velocity at the outer edge of the current zone (km s^{-1}), inward gravitational acceleration (cm s^{-2}), total outward radiative acceleration (cm s^{-2}), and the fraction of this acceleration caused by the incident continuum, line driving, and the gradient of the radiation pressure.

[2] CLOUDY defines heating as the energy input by the freed photoelectron, or $h\nu - $IP, where IP is the ionization potential of the atom or ion, and $h\nu$ is the energy of the photon. See AGN3 for more details.

```
P(Lines):(Mg 2  2796A 0.32) (Mg 2  2803A 0.20) (H  1  6563A 0.13) (H  1 1.875m 0.10) (Fe 2  1786A 0.06) (H  1  4861A 0.05)
```

A line describing the source of the radiation pressure is generated if the ratio of line radiation to gas pressure, P_{rad}/P_{gas}, is greater than 5%. The line begins with the label "P(Lines)" and continues with the fraction of the total radiation pressure produced by that emission line, the spectroscopic designation of the line, and its wavelength. Up to twenty lines can be printed, although in most cases only Lα and a few others will dominate.

```
 Hydrogen      2.15e-04 1.00e+00 H+o/Hden 1.00e+00 1.00e-11 H-    H2 5.27e-19 3.99e-13 H2+ HeH+ 2.03e-14 Ho+ ColD 2.38e+14 1.11e+18
 Deuterium     2.15e-04 1.00e+00 D+o/Dden 1.00e+00 5.61e-12 D-    HD 6.70e-16 2.92e-12 HD+ HeD+ 1.40e-14 Do+ ColD 3.93e+09 1.83e+13
```

The line begins with the ratios $n(\mathrm{H}^0)/n(H_{tot})$ and $n(\mathrm{H}^+)/n(\mathrm{H}_{tot})$ where H_{tot} is the total density in H all forms (including molecular). If **print h-like departure coefficients** has been specified then departure coefficients are also printed on the following line. Neutral hydrogen H^0 is defined to be the total population of atomic hydrogen in all explicitly computed bound levels. Next comes "H+o/Hden", the ratio $[n(\mathrm{H}^0)+n(\mathrm{H}^+)]/n(\mathrm{H}_{tot})$.

The following five numbers give densities of the negative hydrogen ion and several molecules (H^-, H_2, H_2^+, and HeH^+) relative to the total hydrogen density. Note that, with this definition of the hydrogen density, a fully molecular gas will have $n(\mathrm{H2})/n(\mathrm{H}) = 0.5$. These molecular abundances are also expressed as departure coefficients if the **print departure coefficients** command occurs. The last number is the H^0 and H^+ column densities (cm^{-2}).

The next line gives very similar information for deuterium.

```
 H  1 1S-12    1.39e-01 3.43e-04 1.02e-03 1.02e-03 1.24e-03 1.62e-03 2.12e-03 2.73e-03 3.43e-03 4.23e-03 5.12e-03 6.12e-03 7.20e-03
 H  1  rest    8.39e-03 9.66e-03 1.10e-02 1.25e-02 1.41e-02 1.57e-02 1.75e-02 1.93e-02 2.13e-02 2.33e-02 2.54e-02 2.77e-02 3.00e-02
               3.24e-02 3.49e-02 3.75e-02 4.02e-02 4.30e-02 4.59e-02 4.89e-02 5.20e-02 5.51e-02 5.84e-02 6.18e-02 6.52e-02 6.88e-02
               7.24e-02 7.62e-02 8.00e-02 8.39e-02 8.79e-02 9.21e-02 9.63e-02 1.01e-01 1.05e-01 1.09e-01 1.14e-01 1.19e-01
```

This information is only printed if the **print H-like populations** command occurs. The numbers give the populations of the H^0 levels relative to the ionized hydrogen density. All of these populations usually are relative to the ionized hydrogen density, but can also be printed as LTE departure coefficients if the **print departure coefficients** command is given.

```
Helium        6.57e-04 9.45e-01 5.47e-02 He I2SP3 3.52e-06 Comp H,C 1.75e-22 4.64e-23 Fill Fac 1.00e+00 Gam1/tot 1.00e+00
```

The first three numbers are the total populations of the three ionization stages of helium relative to the total helium abundance. The population of atomic helium is the sum of the total population in the triplets and singlets, including the population of all explicitly computed levels of each. These populations can also be expressed as departure coefficients if this option is set with the **print departure coefficients** command. The population of He 2^3 S, relative to the total helium abundance, follows. The Compton heating and cooling rates (both erg cm^{-3} s^{-1}) are next, followed by the gas filling factor. The last number is the fraction of the total hydrogen ionizations that are caused by photoionization from the ground state.

```
He singlet n  6.54e-04 2.35e-11 6.59e-18 2.09e-18 3.18e-18 2.52e-18 He tripl 3.52e-06 9.32e-16 7.41e-18 4.77e-17 7.56e-18
```

The first numbers are the level populations of the l-levels within $n = 1$ to 3 of the He^0 singlets. The next group consists of He^0 triplet populations of $2S$, the three 2^3P_j, levels and the $3S$, $3P$, and $3D$ levels. All populations are relative to the total helium abundance. Departure coefficients are also printed if requested.

```
Pressure      NgasTgas 2.06e+08 P(total) 2.84e-08 P( gas ) 2.84e-08 P(Radtn) 1.79e-11 Rad accl 3.51e-05 ForceMul 3.33e+03
              Texc(La) 4.21e+03 T(contn) 4.59e+01 T(diffs) 2.03e+00 nT (c+d) 1.16e+07 Prad/Gas 6.30e-04 Pmag/Gas 2.80e-04
```

Some information concerning the pressure is printed. The gas equation of state includes thermal gas pressure, the radiation pressure due to trapped line emission, magnetic and turbulent pressure, and the radiation pressure due to absorption of the incident continuum. The first number is the gas pressure $n_{gas}T_{gas}$ (with units cm^{-3} K), followed by the total pressure (dynes cm^{-2}), and is followed by the gas pressure $(n_{gas}kT_{gas})$ in dynes cm^{-2}. The radiation pressure follows. The second to last number is the radiative acceleration (cm s^{-2}) at the inner edge of this zone. The radiative acceleration is computed with all continuous scattering and absorption opacities included. The last number is a force multiplier, defined as in Tarter and McKee (1973), and is the ratio of total opacity to electron scattering opacity.

The second line gives more information. The line starts with "Texc(La)", the excitation temperature T_{exc} of Lα, defined as

$$\frac{n(2p)/g(2p)}{n(1s)/g(1s)} = \exp\left[-h\nu/kT_{exc}(L\alpha)\right]. \tag{1.8}$$

This is followed by the temperature corresponding to the energy density of the attenuated incident continuum ("T(contn)") and the diffuse continua ("T(diffs)"). This includes all trapped lines and diffuse continuous emission. The entry "nT (c+d)"is the energy density of the sum of these two continua expressed as an equivalent pressure nT [cm^{-3} K]. The line ends with the ratios of the radiation to gas pressure "Prad/Gas" and the ratio of magnetic to gas pressure "Pmag/Gas".

```
gra-orion01*  DustTemp 2.12e+02 Pot Volt 5.32e+00 Chrg (e) 1.21e+02 drf cm/s 4.83e+03 Heating: 4.26e-18 Frac tot 1.23e-02
gra-orion02*  DustTemp 2.02e+02 Pot Volt 5.08e+00 Chrg (e) 1.43e+02 drf cm/s 5.26e+03 Heating: 3.69e-18 Frac tot 1.07e-02
gra-orion03*  DustTemp 1.91e+02 Pot Volt 4.86e+00 Chrg (e) 1.70e+02 drf cm/s 5.60e+03 Heating: 3.21e-18 Frac tot 9.26e-03
gra-orion04*  DustTemp 1.81e+02 Pot Volt 4.66e+00 Chrg (e) 2.01e+02 drf cm/s 5.86e+03 Heating: 2.79e-18 Frac tot 8.06e-03
gra-orion05   DustTemp 1.70e+02 Pot Volt 4.47e+00 Chrg (e) 2.39e+02 drf cm/s 6.07e+03 Heating: 2.43e-18 Frac tot 7.03e-03
gra-orion06   DustTemp 1.60e+02 Pot Volt 4.30e+00 Chrg (e) 2.85e+02 drf cm/s 6.22e+03 Heating: 2.13e-18 Frac tot 6.16e-03
gra-orion07   DustTemp 1.50e+02 Pot Volt 4.15e+00 Chrg (e) 3.40e+02 drf cm/s 6.33e+03 Heating: 1.87e-18 Frac tot 5.41e-03
gra-orion08   DustTemp 1.40e+02 Pot Volt 4.02e+00 Chrg (e) 4.07e+02 drf cm/s 6.42e+03 Heating: 1.65e-18 Frac tot 4.77e-03
gra-orion09   DustTemp 1.31e+02 Pot Volt 3.91e+00 Chrg (e) 4.89e+02 drf cm/s 6.48e+03 Heating: 1.46e-18 Frac tot 4.21e-03
gra-orion10   DustTemp 1.22e+02 Pot Volt 3.80e+00 Chrg (e) 5.89e+02 drf cm/s 6.54e+03 Heating: 1.29e-18 Frac tot 3.73e-03
sil-orion01*  DustTemp 1.55e+02 Pot Volt 2.85e+00 Chrg (e) 6.44e+01 drf cm/s 1.45e+04 Heating: 2.44e-18 Frac tot 7.06e-03
sil-orion02*  DustTemp 1.49e+02 Pot Volt 2.70e+00 Chrg (e) 7.58e+01 drf cm/s 1.62e+04 Heating: 2.09e-18 Frac tot 6.03e-03
sil-orion03*  DustTemp 1.43e+02 Pot Volt 2.57e+00 Chrg (e) 8.92e+01 drf cm/s 1.77e+04 Heating: 1.78e-18 Frac tot 5.15e-03
sil-orion04   DustTemp 1.37e+02 Pot Volt 2.44e+00 Chrg (e) 1.05e+02 drf cm/s 1.91e+04 Heating: 1.53e-18 Frac tot 4.42e-03
sil-orion05   DustTemp 1.31e+02 Pot Volt 2.33e+00 Chrg (e) 1.24e+02 drf cm/s 2.02e+04 Heating: 1.32e-18 Frac tot 3.81e-03
sil-orion06   DustTemp 1.26e+02 Pot Volt 2.24e+00 Chrg (e) 1.47e+02 drf cm/s 2.11e+04 Heating: 1.14e-18 Frac tot 3.30e-03
sil-orion07   DustTemp 1.20e+02 Pot Volt 2.15e+00 Chrg (e) 1.76e+02 drf cm/s 2.18e+04 Heating: 9.93e-19 Frac tot 2.87e-03
sil-orion08   DustTemp 1.15e+02 Pot Volt 2.08e+00 Chrg (e) 2.10e+02 drf cm/s 2.23e+04 Heating: 8.67e-19 Frac tot 2.50e-03
sil-orion09   DustTemp 1.10e+02 Pot Volt 2.01e+00 Chrg (e) 2.52e+02 drf cm/s 2.26e+04 Heating: 7.60e-19 Frac tot 2.20e-03
sil-orion10   DustTemp 1.06e+02 Pot Volt 1.96e+00 Chrg (e) 3.03e+02 drf cm/s 2.28e+04 Heating: 6.69e-19 Frac tot 1.93e-03
pah-bt9401 *  DustTemp 3.41e+02 Pot Volt 6.60e+00 Chrg (e) 1.06e+00 drf cm/s 1.97e+02 Heating: 9.29e-22 Frac tot 2.68e-06
pah-bt9402 *  DustTemp 3.44e+02 Pot Volt 6.64e+00 Chrg (e) 1.28e+00 drf cm/s 2.13e+02 Heating: 1.01e-21 Frac tot 2.92e-06
pah-bt9403 *  DustTemp 3.47e+02 Pot Volt 6.61e+00 Chrg (e) 1.49e+00 drf cm/s 2.37e+02 Heating: 1.07e-21 Frac tot 3.08e-06
pah-bt9404 *  DustTemp 3.50e+02 Pot Volt 6.54e+00 Chrg (e) 1.70e+00 drf cm/s 2.67e+02 Heating: 1.09e-21 Frac tot 3.16e-06
pah-bt9405 *  DustTemp 3.53e+02 Pot Volt 6.44e+00 Chrg (e) 1.92e+00 drf cm/s 3.02e+02 Heating: 1.09e-21 Frac tot 3.16e-06
pah-bt9406 *  DustTemp 3.55e+02 Pot Volt 6.45e+00 Chrg (e) 2.22e+00 drf cm/s 3.29e+02 Heating: 1.13e-21 Frac tot 3.26e-06
pah-bt9407 *  DustTemp 3.57e+02 Pot Volt 6.47e+00 Chrg (e) 2.54e+00 drf cm/s 3.60e+02 Heating: 1.17e-21 Frac tot 3.38e-06
pah-bt9408 *  DustTemp 3.59e+02 Pot Volt 6.43e+00 Chrg (e) 2.87e+00 drf cm/s 4.00e+02 Heating: 1.18e-21 Frac tot 3.40e-06
pah-bt9409 *  DustTemp 3.61e+02 Pot Volt 6.46e+00 Chrg (e) 3.27e+00 drf cm/s 4.35e+02 Heating: 1.20e-21 Frac tot 3.46e-06
pah-bt9410 *  DustTemp 3.63e+02 Pot Volt 6.48e+00 Chrg (e) 3.71e+00 drf cm/s 4.74e+02 Heating: 1.22e-21 Frac tot 3.52e-06
```

Some properties of the grain populations are printed if they are present. Each line gives the results of calculations for a specific type and size of grain. Graphite and silicate are normally included when grains are present. Each line begins with the name of the grain and an asterisk appears if quantum heating was important for the species. Quantum heating is only computed if it is significant due to its computational expense. The remainder of the line gives the equilibrium temperature of the grain, the potential in volts, the charge, the drift velocity, the gas heating (erg cm^{-3} s^{-1}) due to grain electron photoemission, and the dimensionless fraction of the total gas heating due to grain electron photoemission. For quantum-heated grains the temperature is the average weighted by T^4.

```
Molecules     CH/Ctot: 3.65e-04 CH+/Ctot 5.82e-13 CO/Ctot: 5.52e-01 CO+/Ctot 1.95e-14 H2O/Otot 3.27e-09 OH/Ototl 4.18e-11
```

A line giving relative abundances of some molecules is printed if the molecular fraction is significant. All molecular abundances are relative to either the total carbon or total oxygen abundance (this is indicated in the label for each). In order, the molecules are CH, CH^+, CO, CO^+, H_2O, and OH.

```
Lithium       8.94e-02 9.11e-01 9.53e-10 0.00e+00 Berylliu 9.99e-01 6.40e-04 6.38e-05 7.06e-10 0.00e+00 sec ion: 7.66e-15

Abundances of each stage of ionization of lithium and beryllium relative
to the total gas-phase abundance of the element are followed by the
suprathermal secondary ionization rate [s$^{-1}$].
{\setverbatimfontsize{\tiny}
\begin{verbatim}
Carbon        6.76e-07 1.91e-02 9.70e-01 1.10e-02 1.77e-04 2.36e-09 0.00e+00 H2O+/O   0.00e+00 OH+/Otot 0.00e+00 Hex(tot) 0.00e+00
```

The abundances of the seven stages of ionization of carbon relative to the total gas-phase carbon abundance begin the line. The abundance of H_2O^+ and OH^+ relative to the total gas-phase oxygen abundance are given. These are followed by "Hex(tot)", the extra heat (erg cm^{-3} s^{-1}) due to fast neutrons, dissipation of turbulence, or added with the **hextra** command.

```
Nitrogen      1.60e-06 1.72e-02 9.69e-01 1.41e-02 4.77e-05 1.34e-07 9.81e-14 0.00e+00 O2/Ototl 0.00e+00 O2+/Otot 0.00e+00
```

The relative populations of the eight ionization stages of nitrogen are printed first. The abundance of O_2 and O_2^+, relative to the total oxygen abundance, follows.

```
 Silicon    0  1.13e-07 8.39e-03 8.16e-01 1.56e-01 1.86e-02 4.68e-05 3.08e-08 5.13e-12 1.63e-16 0.00e+00 0.00e+00 0.00e+00 0.00e+00
 Sulphur    0  7.25e-08 7.46e-03 9.03e-01 8.81e-02 1.60e-03 1.67e-04 5.91e-06 9.11e-10 3.49e-14 3.20e-19 0.00e+00 0.00e+00 0.00e+00
 Chlorine   0  2.51e-07 1.32e-02 9.57e-01 2.92e-02 7.57e-04 5.50e-05 7.07e-07 9.54e-09 2.94e-13 2.17e-18 0.00e+00 0.00e+00 0.00e+00
 Argon      1  9.50e-08 2.83e-03 9.69e-01 2.73e-02 4.35e-04 2.65e-05 3.24e-07 1.53e-09 1.16e-11 8.21e-17 0.00e+00 0.00e+00 0.00e+00
 Iron       3  1.78e-08 2.88e-04 1.08e-01 8.56e-01 3.26e-02 2.33e-03 2.33e-05 2.30e-07 1.28e-10 1.94e-14 9.07e-19 0.00e+00 0.00e+00
```

There are too many ionization stages to print across the line for elements more massive than neon. Although all stages with non-trivial abundances are computed, only the highest twelve stages of ionization are printed. The first number is an integer indicating how many stages are "off the page to the left". If the number is 2, then the first printed stage of ionization is twice ionized, i.e., Fe^{+2}.

1.6 Comments after the calculation

```
    the Orion HII Region / PDR / Molecular cloud with an open geometry
   Calculation stopped because outer radius reached. Iteration 1 of 2
```

A series of messages appear after the printout of the last zone. The first will say why the calculation stopped. In a valid calculation the model will stop because one of the specified stopping criteria specified was met. If no other criteria are specified then the calculation usually stops when the default lowest temperature of 4000 K is reached. If the code stops because of an unintended reason (i.e., internal errors, or reaching the default limit to the number of zones) then a warning is printed saying that the calculation may have halted prematurely.

Only one stopping criterion message will be printed. The possible messages, and their interpretations, are:

...because of radiation pressure By default a cloud will have constant density. CLOUDY will keep the total pressure, particle and radiation, constant if constant pressure is specified with the **constant pressure** command. The radiation pressure is small at the boundaries of the cloud, so the cloud will be unstable if the ratio of radiation to total pressure exceeds 0.5. The calculation stops, and this message is generated, if $P_{rad}/P_{tot} > 0.5$ occurs after the first iteration.

...because lowest EDEN reached The calculation can be forced to stop when the electron density (**eden**) falls below the value set by the **stop eden** command. This can be used to stop the calculation at an ionization front. The default lowest electron density is negative, so this stopping criterion occurs only when the command is entered.

...because low electron fraction The calculation can be forced to stop when the ratio of electron to hydrogen densities falls below a certain value, as set by the **stop efrac** command. This can be used to stop the calculation at an ionization front when the hydrogen density there is not known (for instance, in a constant pressure model). The default lowest electron density is negative, so this stopping criterion applies only when the command is entered.

...because large H_2/H fraction The calculation can be forced to stop when the ratio of densities of molecular hydrogen to total hydrogen rises above the value set by the **stop mfrac** command. The molecular fraction is defined as $2n(H_2)/n(H_{tot})$. This can be used to stop the calculation at some depth into a PDR. The default highest molecular density is $>> 1$, so this stopping criterion occurs only when the **stop mfrac** command is entered.

...because wind veloc too small The code can perform a wind calculation which includes the outward force due to radiation pressure and the inward force of gravity. This message is printed if the gas decelerates to a stop.

...because code returned BUSTED The calculation stopped because something bad happened. Please post the input script and version number on the discussion board.

...because DRAD small - set DRMIN The Strömgren radius of the H^+ zone is estimated at the start of the calculation and the smallest allowed zone thickness is set to a very small fraction of this. The calculation will stop if the zone thickness falls below this smallest thickness. This can occur because of any of several logical errors within CLOUDY (adaptive logic is used to continuously adjust the zone thickness), although it can rarely occur for physical reasons as well. The smallest thickness can be reset to any number with the set **drmin** command but it should not be necessary to do this. Please post the input script and version number on the discussion board.

...because DR small rel to thick The depth into the cloud is stored as the double precision variable *depth* and the zone thickness is stored as the double precision variable *drad*. If the zone size becomes too small relative to the depth (*drad/depth* $< 10^{-14}$) then the depth variable will underflow such that *depth* + *drad* = *depth*. The calculation will stop if this problem prevents the density from being properly evaluated.

...because optical depth reached The largest allowed continuous absorption optical depth can be set with the **stop optical depth** command. The command specifies both the absorption optical depth, and the energy at which it is to be evaluated. Scattering opacities are not included since their effects are very geometry dependent. If the calculation stops because the largest continuum optical depth is reached, then this line is printed. This line is also printed if the **stop effective column density** command is used to stop the calculation, since this command is actually a form of the **stop optical depth** command.

...because outer radius reached The default outer radius is unphysically large, but can be changed with the **radius** or **stop thickness** commands. If the calculation stops because the outer radius set by one of these commands is reached, then this line is printed.

because column dens reached a limit to the largest allowed neutral, ionized, and total hydrogen column densities is set with the **stop column density**, **stop neutral column density**, or **stop ionized column density** commands. This message will be printed if one of these criteria stops the calculation.

...because lowest Te reached The default value of the lowest temperature allowed is 4000 K. This is reasonable when only emission from warm ionized gas is of interest. The limit can be changed with the **stop temperature** command. This message is printed if the calculation stops because the lowest temperature is reached.

...because highest Te reached The default value of the highest temperature allowed is 1.001×10^{10} K. The limit can be changed with the **stop temperature exceeds** command. This message is printed if the calculation stops because the highest allowed temperature is exceeded.

...because freeze out fraction Nick Abel incorporated the condensation of molecules onto grain surfaces. Currently CO, H_2O, and OH condensation are treated. The chemistry network will become unstable when oxygen is highly depleted from the gas phase. By default the code stops when 99% of the oxygen abundance has condensed out of the gas phase.

...because NZONE reached By default the code will stop after computing 1400 zones. This can be reset with the **stop zone** command. This message is printed if the calculation stops because the limiting number of zones is reached. A warning is printed at the end of the calculation since this was probably not intended.

The default limit to the number of zones can be increased, while retaining the check that the default limit is not hit, by using the **set nend** command.

...because volume too large for this cpu This indicates that the effective volume of the last zone was too large to be represented as a single precision floating point number. This happens when $R/R_{\rm in}$ becomes really large. Usually this indicates that none of the intended stopping criteria were hit, so you should check those. If you really intend for the simulation to integrate this far, you should increase the inner radius.

...because line ratio reached It is possible to set a limit to the largest value of an emission-line intensity ratio with the **stop line** command. This message is printed if the calculation stops because the largest value of the ratio is reached.

...because internal error - DRAD An internal logical error caused this message to be printed. Please report the problem, including the command lines and the version number of CLOUDY, on the discussion board at the code's web site, .

...because initial conditions out of bounds The temperature of the first zone was not within the temperature bounds of the code. This is probably due to the incident continuum not being set properly.

...because zero electron density The electron density fell to zero because there was no source of ionization. This is unphysical and usually occurs because the cloud boundary conditions were not set properly. Consider adding at least galactic background cosmic rays with the **cosmic ray background** command and perhaps the galactic or extragalactic background.

...because reason not specified This is an internal error. Please post the input and version number on the code's discussion board.

1.7 Geometry

```
The geometry is plane-parallel.
```

The code will next say whether the geometry is plane parallel ($\Delta r/r_o < 0.1$), a thick shell ($\Delta r/r_o < 3$), or spherical ($\Delta r/r_o \geq 3$), where r_o is the inner radius and Δr is the thickness of the cloud.

1.8 Warnings, Cautions, Surprises, and Notes

```
C-Cloud thicker than smallest Jeans length=3.51e+16cm; stability problems? (smallest Jeans mass=2.58e-01Mo)
 !Magnetic field & cosmic rays both present.  Their interations are not treated.
 !Some input lines contained underscores, these were changed to spaces.
 !Suprathermal collisional ionization of H reached 83.84% of the local H ionization rate.
 !H2 vib deexec heating reached 6.68% of the local heating.
 !Charge transfer ionization of H reached 95.8% of the local H ionization rate.
 !The largest continuum brightness temperature was 4.835e+05K at 1.052e-08 Ryd.
 !Both constant pressure and turbulence makes no physical sense???
 !AGE: Cloud age was not set.  Longest timescale was 8.43e+15 s = 2.67e+08 years.
 !The excitation temp of Lya exceeded the electron temp, largest value was  4.60e+03K (gas temp there was  1.01e+03K, zone 310)
 !Line absorption heating reached 13.45% of the local heating - largest by level 1 line Si 2 34.8m
 !Some infrared fine structure lines are optically thick:  largest tau was  2.05e+03
 !Local grain-gas photoelectric heating rate reached  98.8% of the total.
 !The local H2 photodissociation heating rate reached 12.8% of the total heating.
 !The CMB was not included.  This is added with the CMB command.
 !The fraction of H  in H2    reached 100.0% at some point in the cloud.
 !The fraction of C  in CO     reached 100.0% at some point in the cloud.
 !The fraction of N  in N2     reached 99.7% at some point in the cloud.
 !The fraction of S  in CS     reached 100.0% at some point in the cloud.
 !The fraction of S  in SO     reached 56.9% at some point in the cloud.
 !The fraction of S  in OCS    reached 36.3% at some point in the cloud.
 !The fraction of Cl in HCl    reached 24.5% at some point in the cloud.
 !The fraction of O  in H2Ogrn reached 58.3% at some point in the cloud.
 !A signficant amount of molecules condensed onto grain surfaces.
 !These are the molecular species with "grn" above.
 !The optical depth in the H I 21 cm line is 6.84e-01
 !The optical depth in the 12CO J=1-0 line is 2.79e+05
 !The radiation pressure jumped by 123% at zone 334, from 5.28e-11 to 3.67e-11 to 3.73e-11
 !The H2 density varied by 12.6% between two zones
  Continuum fluorescent production of H-beta was significant.
  Te-ne bounds of Case B lookup table exceeded, H I Case B line intensities set to zero.
  Te-ne bounds of Case B lookup table exceeded, He II Case B line intensities set to zero.
  Destruction of He 2TriS reached 3.4% of the total He0 dest rate at zone 236, 3.4% of that was photoionization.
  Critical density for l-mixing of He I not reached.  More resolved levels are needed for accurate He I line ratios.
  The largest continuum occupation number was 2.911e+08 at 1.052e-08 Ryd.
  The continuum occupation number fell below 1 at 1.944e+04 microns.
  The continuum brightness temperature fell below 10000K at 1.433e+06 microns.
  Ratio of computed diffuse emission to case B reached 2.30168 for iso 1 element 2
  Global grain photoelectric heating of gas was  9.9% of the total.
  Local grain-gas cooling of gas rate reached  90.4% of the total.
  The local H2 cooling rate reached 7.2% of the local cooling.
  Local CO rotation cooling reached 83.0% of the local cooling.
  The Balmer continuum optical depth was  3.68e+03.
  The Balmer continuum stimulated emission correction to optical depths reached  7.64e-02.
  The Paschen continuum optical depth was 1.69e+03.
  The continuum optical depth at the lowest energy considered (1.052e-08 Ryd) was  3.213e+03.
  The optical depth to Rayleigh scattering at 1300A is 4.36e-02
  3 body rec coef outside range 1
  The fraction of Cl in CCl+   reached 0.103% at some point in the cloud.
  The fraction of N  in HNC    reached 0.312% at some point in the cloud.
  The fraction of C  in C2H    reached 2.60% at some point in the cloud.
  The fraction of C  in COgrn  reached 0.379% at some point in the cloud.
```

The next messages fall into four categories: warnings beginning with “W-”; cautions beginning with “C-”; surprising results beginning with an explanation mark (“!”), and notes.

CLOUDY does many internal sanity checks to confirm that its range of validity was not exceeded (Ferland, 2001a). Warnings are issued to indicate that the program has not treated an important process correctly. For instance, warnings occur if the temperature was high enough for the electrons to be relativistic, if the global heating - cooling balance is off by more than 20%, or if the code stopped for an unintended reason. We would like to hear about warnings - the web site has a discussion board to place comments. Cautions are less severe, and indicate that CLOUDY is on thin ice. Examples are when the optical depths in excited states of hydrogen change during the last iteration. Surprises indicate that, while the physical process has been treated correctly, the result is surprising. An example is when induced Compton heating is more that 5 percent of the total Compton heating. Notes indicate interesting features about the model, such as maser effects in lines or continua, or if the fine structure lines are optically thick. The messages are usually self-explanatory.

1.9 Optional Plot

```
l-                                  l                                   l                                  o
-------------------------------------------------------------------------------------------------------------o-
 0.1                                1                                  10
```

If any of the optional plots are requested with a **plot - -** command then they will appear next. This option is seldom used today since it is much easier to create data files with save commands and then use other software to make plots.

1.10 Final Printout

```
                ********************************> Cloudy 06.01.02 <********************************
                * title the Orion HII Region / PDR / Molecular cloud with an open geometry        *
                * #                                                                              *
                * # commands controlling continuum =========                                     *
        -
        -
        -
        -
                * assert line luminosity "12CO" 235.4m  -2.80 error 0.15                        *
                * assert line luminosity "12CO" 215.7m  -2.84 error 0.15                        *
                * assert nzone < 1400                                                           *
                * assert itrzn < 24                                                             *
                * # orion hii pdr pp.in                                                         *
                * # class hii pdr                                                               *
                * # ========================================                                     *
                ********************************> Log(U): -1.48 <*********************************
                >>>>>>>>>> Cautions are present.
```

The final printout begins by reprinting the input commands. The box surrounding it gives both the version number of CLOUDY (at the top) and the log of the ionization parameter (the ratio of ionizing photon to hydrogen densities) at the bottom.

```
Emission Line Spectrum.  Constant  Pressure Model.    Open geometry.  Iteration 2 of 2.
                                Intensity (erg/s/cm^2)
```

This line summarizes some properties of the model and output. The first part indicates whether the energy in the emission lines is given as the luminosity case (the energy radiated by a spherical shell covering Ω sr [erg s^{-1}] where $\Omega/4\pi$ is the covering factor) or the intensity case (emission produced by a unit area of gas [erg s^{-1} cm^{-2}])). Which of the two choices is printed is determined by whether the luminosity of the continuum was specified as the luminosity radiated by the central object into 4π sr or the intensity $(4\pi J)$ of the incident continuum (erg cm^{-2} s^{-1}) at the illuminated face of the cloud. If the cloud is spherical and the intensity case is computed then the emergent emission-line spectrum will be per unit area in units of the inner radius ro (that is, the total line luminosity radiated by a shell covering 4π sr will be the listed intensity $4\pi J \times 4\pi r_o^2$). The second part of this line indicates the density structure (i.e., wind, constant density, constant pressure, constant gas pressure, power-law density distribution, etc). The next section tells whether the geometry was open or closed (these are defined in Part I of this document). The last part indicates the iteration number.

```
                                                Intrinsic line intensities
 general properties.....        H  1 1.500m  -2.042   0.0010      +Col 1.278m  -1.666   0.0024      O  2 833.8A  -1.615   0.0027
 H  1  4861A   0.473   0.3311      H  1 7.458m  -1.094   0.0090      Ca B 1.870m  -1.760   0.0019      O 2r  4651A  -2.135   0.0008
 H  1  1216A   0.740   0.6119      H  1 4.653m  -1.299   0.0056      +Col 1.870m  -1.757   0.0019      O 2r  4341A  -2.413   0.0004
 Inci     0    3.001 111.7791      H  1 3.740m  -1.487   0.0036      Ca B 1.279m  -2.153   0.0008      TOTL  4341A  -2.413   0.0004
 TotH     0    1.727   5.9400      H  1 3.296m  -1.650   0.0025      +Col 1.279m  -2.149   0.0008      TOTL  1665A  -1.363   0.0048
-
 -
 -
 H  1 1.513m  -2.287   0.0006      Ca B 1.869m  -1.283   0.0058      O 2r  2471A  -2.363   0.0005      hyperfine structure.........
 H  1 1.508m  -1.964   0.0012      +Col 1.869m  -1.275   0.0059      O 2r  7323A  -2.536   0.0003      inner shell.................
 H  1 1.504m  -1.999   0.0011      Ca B 1.278m  -1.676   0.0024      O 2r  7332A  -2.657   0.0002
                                                Emergent line intensities
 H  1  4861A   0.132   1.0000      12CO 517.8m  -3.749   0.0001      12CO 431.5m  -3.474   0.0002      12CO 369.8m  -3.268   0.0004
 13CO 353.6m  -3.709   0.0001      13CO 309.4m  -3.605   0.0002      13CO 275.0m  -3.547   0.0002      13CO 247.5m  -3.544   0.0002
```

```
 13CO 225.0m  -3.641   0.0002      H  1  1216A   0.547   2.6028          H  1  1026A  -1.178   0.0490      H  1 972.5A  -1.350   0.0330
-
-
-
 C  3 398.4A  -3.773   0.0001      N  1 980.7A  -3.567   0.0002      N  2 916.3A  -2.513   0.0023      N  2 646.4A  -2.307   0.0036
 N  3 348.7A  -3.763   0.0001      O  1  7950A  -2.869   0.0010      O  2  4188A  -3.756   0.0001      O  2 386.3A  -1.774   0.0124
 O  2 385.7A  -1.955   0.0082      O  3 300.5A  -3.653   0.0002
```

A series of predicted quantities follow. These are mainly emission-line intensities although the output also includes other predicted quantities.

Some continua and various indications of contributors to lines and continua are included. The Chapter of this document describing observed quantities (starting on page 25) tells how to convert these into some observed quantities. Not all are printed by default. The discussions on the **print** commands in Part I tell how to get more or fewer predictions. This list of emission lines can also be sorted by wavelength or intensity, and can be printed as a single column so that they can be entered into a spreadsheet.

The organization and meaning of the different of lines in the printout is discussed in the Chapter *The Emission Lines* starting on page 95.

A list of emission lines with negative relative intensities may follow the main block of lines. These are lines which heat rather than cool the gas (heating is negative cooling). This is not a problem but occurs if the line's collisional de-excitation rate exceeds its collisional excitation rate. This usually occurs when the line is radiatively excited but collisionally de-excited.

1.10.1 Intrinsic line intensities and luminosities

There are two blocks of predicted intensities. The block "Intrinsic line intensities" is the intrinsic emission from the cloud. The intrinsic emission includes all processes that affect the line formation and transfer. This includes collisional processes, fluorescence, line destruction by background opacities such as dust or the Lyman continuum of hydrogen, and recombination. The intrinsic intensities do not include the effects of absorbers or scatters that do not lie within the line-formation region.

1.10.2 Emergent line intensities and luminosities

The block "Emergent line intensities" is the emission observed from outside the cloud. In an open geometry the inward part of the line includes the effects of extinction between the line-forming region and the illuminated face. There is an additional contribution due to reflection off the gas in the outward direction. The outward part of the line includes the effects of extinction between the shielded face and the point where the line forms. In a closed geometry the emergent intensity is the emission escaping to the outer edge of the slab. All of this is very geometry dependent. For an open geometry, in particular, the observed emission will depend strongly upon the viewing angle.

If the intrinsic and emergent values are very different then it is important to understand the geometry and what is actually observed. This is an indication of the uncertainty if the predictions have a strong geometry dependence.

The following is an example of the emission-line output. The first column indicates the species and the second is the wavelength. "A" indicates angstrom and "m" indicates micron. The third column is the log of the intensity [erg cm^{-2} s^{-1}] or luminosity [erg s^{-1}] depending on which case was used. The last column is the intensity of the line relative to the normalization line, Hβ by default.

```
Blnd      4725.00A  -17.316    0.1805
Ar 4      4740.12A  -17.639    0.0858
He 2      4859.18A  -17.839    0.0541
H  1      4861.33A  -16.572    1.0000
Fe 7      4893.37A  -18.376    0.0157
He 1      4921.93A  -19.511    0.0012
Fe 7      4942.48A  -18.787    0.0061
O  3      4958.91A  -16.542    1.0722
Fe 6      4967.15A  -17.661    0.0815
Fe 6      4972.48A  -17.239    0.2153
Fe 7      4988.55A  -18.106    0.0293
Pcon      5000.00A    1.373 *********
O  3      5006.84A  -16.067    3.1990
Blnd      5007.00A  -15.942    4.2715
O3bn      5007.00A   -0.164 *********
Fe 6      5097.82A  -19.193    0.0024
```

1.10.3 Air vs vacuum wavelengths

The emission line wavelengths follow the convention that vacuum wavelengths are used for $\lambda_{\rm vac} \leq 2000$ Å and STP air wavelengths are used for $\lambda_{\rm vac} > 2000$ Å. The **print line vacuum** command tells the code use use vacuum wavelengths throughout. The continuum is always reported in vacuum wavelengths to avoid a discontinuity at 2000Å.

1.10.4 Some physical properties of the cloud

```
the Orion HII Region / PDR / Molecular cloud with an open geometry
Cooling:  HFBc     0 :0.110 HFFc     0 :0.077 TOTL  3727A:0.074 O  3  5007A:0.210 O  3  4959A:0.070 S  3  9532A:0.074
Heating:  BFH1     0 :0.817 BFHe     0 :0.074 GrGH     0 :0.099
```

Cooling: This line indicates the fraction of the total cooling (defined here as the energy of the freed photoelectron, see AGN3 Chapter 3) carried by the indicated emission lines. The line label is followed by the ratio of the energy in the line to the total cooling. This is an important indication of the fundamental power-losses governing conditions in the model. The labels used are the same as those in the line array.

Heating: This line indicates the fraction of the total heating produced by various processes. The format is the same as the line giving the cooling.

```
IONIZE PARMET:  U(1-) -1.4764  U(4-): -5.0813  U(sp): -4.46  Q(ion):   -4.574  L(ion)-13.505   Q(low): 15.158      L(low)  1.121
```

The line begins with the log of the H "U(1-)" and He^+ "U(4_)" ionization parameters. The third number "U(sp)" is the log of a spherical ionization parameter often used in spherical geometries, such as H II regions or planetary nebulae. It is defined as

$$U_{sph} = \frac{Q\left(\mathrm{H}^0\right)}{4\pi R_s^2 n_{\mathrm{H}} c} \tag{1.9}$$

where R_s is the Strömgren radius, defined as the point where the hydrogen neutral fraction falls to $\mathrm{H}^0/\mathrm{H} = 0.5$. If no ionization front is present then U_{sph} is evaluated at the outer edge of the cloud. The next two numbers are the log of the number of hydrogen-ionizing photons ($h\nu \geq 1$ Ryd) exiting the nebula "Q(ion)" and the log of the energy in this continuum "L(ion)". The next two

numbers are the equivalent quantities for non-ionizing ($h\nu < 1$ Ryd) radiation. These are either per unit area or by a shell covering 4π sr. These have been corrected for the r^{-2} dilution if per unit area, and so are directly comparable with the numbers given at the start of the calculation.

```
ENERGY BUDGET:  Heat:   1.725  Coolg:   1.725  Error:  0.0%  Rec Lin:   1.462  F-F  H -5.612   P(rad/tot)mx:1.10E-01      R(F Con):1.737e+05
```

This line gives an indication of the energy budget of the nebula. The first number "Heat" is the log of the total heating (in ergs s^{-1}, but again either into 4π sr or cm^{-2}). The second number "Coolg" is the log of the total cooling, in the same units. Cooling is the total energy in collisionally excited lines and part of the recombination energy, but *does not* include recombination lines (AGN3 Chapter 3). The percentage error in the heating-cooling - cooling match "Error" follows. The next numbers give "Rec Lin", the log of the total luminosity in recombination lines, "F-F H", the log of the amount of energy deposited by free-free heating, and "P(rad/tot)mx", the largest value of the ratio of radiation to gas pressures that occurred. The line ends with **R(F Con)**, the resolving power in the fine continuum.

```
    Col(Heff):      1.031E+25  snd travl time  5.06E+13 sec  Te-low: 1.69E+01  Te-hi: 1.08E+04 G0TH85:3.54E+05   G0DB96:4.54E+05
```

The effective column density "Col(Heff)", as defined in the section in Part 1 on the **stop effective column density** command, is printed. This is followed by "snd travl time", the sound travel time across the nebula in seconds. Constant pressure is only valid if the cloud is static for times considerably longer than this. The last two numbers are the lowest "Te-low" and highest "Te-hi" electron kinetic temperatures found in the computed structure. The last numbers "G0TH85" and "GHBD96" give the intensity of the ultraviolet radiation field relative to the background Habing value, as defined by Tielens and Hollenbach (1985) and Bertoldi and Draine (1996).

```
 Emiss Measure    n(e)n(p) dl       2.205E+25  n(e)n(He+)dl         1.962E+24  En(e)n(He++) dl      1.402E+21
```

This gives several line-of-sight emission measures. The definition of the line of sight emission measure of a species X is (AGN3 section 5.4)

$$E(X) = \int n(e)\, n(X)\; f(r)\, dr \quad [\mathrm{cm}^{-5}] \tag{1.10}$$

where $f(r)$ is the filling factor. This is given for H^+, He^+, and He^{2+}.

```
He/Ha:9.61E-02  =   1.01*true  Lthin:1.81E+01  itr/zn: 9.78  H2 itr/zn:  0.00  File Opacity: F MassTot  1.12e32  (gm)
```

This line includes some quantities deduced from the predicted emission-line spectrum. The first ("He/Ha") number is the apparent helium abundance He/H, measured from the emission-line intensities using techniques described in AGN3 (Chapter 5);

$$\left(\frac{\mathrm{He}}{\mathrm{H}}\right)_{apparent} = \frac{0.739 \times I(5876) + 0.078 \times I(4686)}{I(\mathrm{H}\beta)}. \tag{1.11}$$

The intensities of all lines are the total predicted intensities and include contributions from collisional excitation and radiative transfer effects. The second number (i.e., "1.07*true") is the ratio of this deduced abundance to the true abundance. This provides a simple way to check whether ionization correction factors, or other effects, would upset the measurement of the helium abundance of the model nebula. This is followed by the longest wavelength in centimeter "Lthin"

at which the nebula is optically thin. Generally the largest FIR opacity source is bremsstrahlung and the number will be 10^{30} if the nebula is optically thin across the full continuum. The number "itr/zn" is the average number of iterations needed to converge each zone while "H2 itr/zn" is the number of iterations per zone required to converge the large H2 model if it is included. "MassTot" gives the total mass of the computed structure in grams if the inner radius was specified. If the inner radius was not specified, and the cloud is plane parallel, then the mass per unit area [gm cm^{-2}] is reported.

```
Temps(21 cm)   T(21cm/Ly a)  8.40E+02       T(<nH/Tkin>)  1.04E+03         T(<nH/Tspin>)   1.29E+03         TB21cm       5.32E+02
               N(H0/Tspin)   5.22E+18       N(OH/Tkin)    2.01E+13
```

This line gives various quantities related to the H I 21 cm line. "T(21cm/Ly a)" gives the temperature deduced from the ratio of the 21 cm to Lα line optical depths (AGN3 Section 5.5). The opacity within the 21 cm line is proportional to $n\left(\mathrm{H}^0\right)\chi/kT$ where χ is the excitation energy of the line. "T(<nH/Tkin>)" gives the harmonic mean temperature

$$\langle T\rangle = \frac{\int Tn\left(\mathrm{H}^0\right)\chi/kT\ dr}{\int n\left(\mathrm{H}^0\right)\chi/kT\ dr} \tag{1.12}$$

where T is the electron or gas kinetic temperature. "T(nH/Tspin)" is the temperature derived from the n/T_{spin} ratio using the 21 cm spin temperature. T_{spin} is calculated from the ratio of populations of the ground fine structure levels, which is computed including the effects of Lα scattering. The spin and kinetic temperatures are often assumed to be equal although they are not in practice. The number "TB21cm" is an estimate of the brightness temperature of the 21 cm line as viewed from the illuminated face of the cloud. It is the spin temperature at a depth where the 21 cm line becomes optically thick at line center.

On the next line the next two numbers are the H^0 and OH column densities divided by the 21 cm spin temperature in the case of H^0 and by the kinetic temperature in the case of OH. These ratios are proportional to the optical depth of a line at radio frequencies.

```
<a>:0.00E+00  erdeFe0.0E+00  Tcompt1.90E+06  Tthr1.19E+13  <Tden>: 2.38E+01  <dens>:2.00E-17 <Mol>:2.31E+00
```

The mean radiative acceleration "<a>" [cm s^{-2}] is printed if the geometry is a wind model and zero otherwise. This is followed by some time scales. "erdeFe" is the time scale, in seconds, to photoerode Fe (Boyd and Ferland, 1987). This is 0s if the γ-ray flux is zero. The next gives the Compton equilibrium timescale "Tcompt" and the thermal cooling timescale "Tthr" [s]. The density (gm cm^{-3}) weighted mean temperature "<Tden>", radius-weighted mean density "<dens>" (gm cm^{-3}), and mean molecular weight "<Mol>", follow.

```
Mean Jeans  l(cm)4.19E+16  M(sun)4.36E-01  smallest:     len(cm):3.53E+16  M(sun):2.61E-01 Alf(ox-tran):     0.0000
```

This gives the mean Jeans length "l(cm)" (cm) and Jeans mass "M(sun)" (in solar units). This is followed by the smallest Jeans length "smallest len(cm)" and the smallest Jeans mass "M(sun)" which occurred in the calculation. The last quantity "Alf(ox-tran)" is the spectral index α_{ox}, defined as in the header, but for the transmitted continuum (attenuated incident continuum plus emitted continuum produced by the cloud).

```
Rion:1.001E+17  Dist:6.17E+21  Diam:6.689E+00
```

This gives the radius of the hydrogen ionization front (in cm), or the outer radius in case the hydrogen ionization front is never reached. This is followed by the distance (in cm), or zero in case the **distance** command was not used. Finally the angular diameter of the ionized region is given (in arcsec), or zero if the distance was not set. The angular diameter is defined as `2*Rion/Dist`.

```
Hatom level 26  NHtopoff:  22  HatomType: add  HInducImp  F  He tot level: 63  He2 level:   26 ExecTime 2233.72
```

This line gives the number of levels of the model hydrogen atom, the "topoff" level, above which the remainder of the recombination coefficient is added, the type of top off used for this calculation, and the number of levels used for the atomic helium. The last number on the line is the execution wall-clock time in seconds.

```
 ConvrgError(%)  <eden>  0.075  MaxEden  0.543  <H-C>   0.20  Max(H-C)    0.50  <Press>   0.042 MaxPres  2.535
  Continuity(%)  chng Te   3.9  elec den   5.8  n(H2)   12.8  n(CO)        8.5
```

The first line gives some estimates of the errors that occurred in several quantities that the code converges. A pair of numbers gives the mean and largest percentage errors for the electron density, the heating-cooling balance, and the pressure. The second line gives the percentage changes that occurred from one zone to the next for the temperature, the electron density, and the H_2 and CO densities.

1.10.5 Average temperatures and densities

```
                                                Averaged Quantities
             Te      Te(Ne)   Te(NeNp)  Te(NeHe+)Te(NeHe2+) Te(NeO+)  Te(NeO2+)  Te(H2)     N(H)     Ne(O2+)   Ne(Np)
Radius:  6.86e+02  9.19e+03  9.27e+03  9.18e+03  9.09e+03  9.65e+03  8.86e+03  2.28e+01  8.30e+06  1.43e+04  1.50e+04
```

This begins with several temperature and density averages, over either radius or volume. The volume averages are only printed if the **sphere** command is entered. The quantity which is printed is indicated at the top of each column. The quantity being averaged is the first part of the label, and the weighting used is indicated by the quantity in parenthesis. For instance "Te(NeO2+)" is the electron temperature averaged with respect to the product of the electron and O^{2+} densities.

```
Peimbert T(OIIIr)9.08E+03 T(Bac)0.00E+00 T(Hth)0.00E+00 t2(Hstrc)  6.01e-03 T(O3-BAC)0.00E+00 t2(O3-BC)  0.00e+00 t2(O3str)  1.81e-03
 Be careful: grains exist.  This spectrum was not corrected for reddening before analysis.
```

This series of quantities deal with temperature fluctuations (t^2, Peimbert, 1967; AGN3 section 5.11) . The code analyzes the predicted emission line and continuum spectrum using the same steps that Manuel outlined in this paper. The code does not attempt to correct the predicted emission-line intensities for collisional suppression or reddening, so this line is only printed if the density is below the density set with the **set tsqden** command—the default is 10^7 cm^{-3}. This code does not attempt to deredden the spectrum: a caution is printed if grains are present.

The nature of temperature fluctuations is, in my option, the biggest open question in nebular astrophysics. Theory (CLOUDY too) predicts that they should be very small because of the steep dependence of the cooling function on the temperature, while some observations indicate a very large value of t^2 (see Liu et al., 1995, Kingdon and Ferland, 1995, and Ferland, 2003). If something is missing from our current understanding of the energy source of photoionized nebulae then the entire nebular abundance scale (for both the Milky Way and the extragalactic nebulae) is in error by as much as 0.5 dex.

Two fundamentally different t^2s enter here—the "structural" t^2 and the "observational" t^2. The structural value comes from the computed ionization and thermal structure of the nebula while the

observational value comes from an analysis of the predicted emission-line spectrum following the methods outlined in Peimbert's 1967 paper.

The structural t^2 for the H^+ ion is defined as

$$t^2\left(H^+\right) = \left\langle \left[\frac{T\left(r\right) - \left\langle T\right\rangle}{\left\langle T\right\rangle}\right]^2 \right\rangle = \frac{\int \left[T\left(r\right) - \left\langle T\right\rangle\right]^2 n_e n\left(H^+\right) f\left(r\right) dV}{\left\langle T\right\rangle^2 \int n_e n\left(H^+\right) f\left(r\right) dV} \tag{1.13}$$

where $< T >$ is the density-volume weighted mean temperature

$$\left\langle T\right\rangle = \frac{\int T\left(r\right) n_e n\left(H^+\right) f\left(r\right) dV}{\int n_e n\left(H^+\right) f\left(r\right) dV}. \tag{1.14}$$

This quantity is given in the averaged quantities block as the column "Te(NeNp)."

The observational t^2—related quantities are the following: "T(OIIIr)" is the electron temperature indicated by the predicted [OIII] 5007/4363 ratio in the low-density limit. This number is meaningless for densities near or above the critical density of the [O III] lines. "T(Bac)" is the hydrogen temperature resulting from the predicted Balmer jump and Hβ. "T(Hth)" is the same but for optically thin Balmer continuum and case B Hβ emission. "t2(Hstrc)" is the structural H II t^2. The entries "T(O3-BAC)" and t2(O3-BC)" are the mean temperature and t^2 resulting from the standard analysis of the [O III] and H I spectra (Peimbert, 1967). Finally "t2(O3str)" is the structural t^2 over the $O2^+$ zone. Only the structural t^2s are meaningful for high densities. This section was developed in association with Jim Kingdon, and Kingdon and Ferland (1995) provide more details.

1.10.6 Average grain properties

```
Average Grain Properties (over radius):
       gra-orion01* gra-orion02* gra-orion03* gra-orion04* gra-orion05* gra-orion06* gra-orion07  gra-orion08  gra-orion09  gra-orion10
    nd:       0            1            2            3            4            5            6            7            8            9
 <Tgr>: 3.659e+01    3.592e+01    3.522e+01    3.450e+01    3.377e+01    3.306e+01    3.236e+01    3.170e+01    3.106e+01    3.045e+01
 <Vel>: 4.177e+02    4.780e+02    5.483e+02    6.279e+02    7.223e+02    8.327e+02    9.572e+02    1.095e+03    1.241e+03    1.396e+03
 <Pot>: 3.072e-01    2.905e-01    2.736e-01    2.575e-01    2.423e-01    2.281e-01    2.151e-01    2.036e-01    1.932e-01    1.842e-01
 <D/G>: 1.202e-04    1.337e-04    1.486e-04    1.653e-04    1.837e-04    2.043e-04    2.271e-04    2.525e-04    2.808e-04    3.122e-04

       sil-orion01* sil-orion02* sil-orion03* sil-orion04* sil-orion05  sil-orion06  sil-orion07  sil-orion08  sil-orion09  sil-orion10
    nd:      10           11           12           13           14           15           16           17           18           19
 <Tgr>: 3.303e+01    3.261e+01    3.216e+01    3.173e+01    3.130e+01    3.090e+01    3.051e+01    3.015e+01    2.981e+01    2.950e+01
 <Vel>: 1.093e+03    1.237e+03    1.385e+03    1.532e+03    1.676e+03    1.817e+03    1.953e+03    2.086e+03    2.215e+03    2.342e+03
 <Pot>: 1.693e-01    1.598e-01    1.509e-01    1.427e-01    1.352e-01    1.283e-01    1.220e-01    1.163e-01    1.109e-01    1.062e-01
 <D/G>: 2.031e-04    2.259e-04    2.511e-04    2.792e-04    3.104e-04    3.451e-04    3.837e-04    4.267e-04    4.744e-04    5.274e-04

       pah-bt9401 * pah-bt9402 * pah-bt9403 * pah-bt9404 * pah-bt9405 * pah-bt9406 * pah-bt9407 * pah-bt9408 * pah-bt9409 * pah-bt9410 *
    nd:      20           21           22           23           24           25           26           27           28           29
 <Tgr>: 4.620e+01    4.634e+01    4.650e+01    4.662e+01    4.675e+01    4.683e+01    4.691e+01    4.697e+01    4.702e+01    4.706e+01
 <Vel>: 9.565e+00    1.100e+01    1.255e+01    1.426e+01    1.617e+01    1.819e+01    2.029e+01    2.261e+01    2.516e+01    2.779e+01
 <Pot>: 2.697e+00    2.424e+00    2.181e+00    1.964e+00    1.768e+00    1.594e+00    1.442e+00    1.307e+00    1.188e+00    1.084e+00
 <D/G>: 9.119e-08    9.556e-08    1.002e-07    1.050e-07    1.100e-07    1.153e-07    1.208e-07    1.266e-07    1.327e-07    1.391e-07
 Dust to gas ratio (by mass): 5.457e-03, A(V)/N(H)(pnt):5.543e-22, (ext):4.024e-22, R:3.647e+00 AV(ext):5.152e+03 (pnt):7.097e+03
```

The next lines give some information concerning grains if these were included in the calculation. These lines give the mean temperature, drift velocity, and potential, for all of the grain populations included in the calculation. An asterisk will appear to the right of the name of any species with quantum heating included. In this case the mean temperature is weighted by T^4.

The last line gives some information related to the grain abundance and optical properties. The first number is the dust to gas ratio by mass. The next two are the total visual extinction per unit hydrogen column density for a point and extended source. These are different because of the different effects of forward scattering (AGN3 section 7.6). Next comes the ratio of total to selective extinction. The line ends with A_V for both an extended and point source.

1.10.7 Optical depths

```
 Contin Optical Depths: COMP: 1.07e-03     H-: 1.90e-04     R(1300): 4.53e-02  H2+: 1.12e-06  Bra:1.55E+02
                        Pa: 7.89e+02    Ba: 3.98e+03      Hb: 5.31e+03    La: 1.07e+04     1r:1.151E+05  1.8:3.79E+07 4.:4.382E+06
  Line Optical Depths: 10830:  8.12e+02  3889: 3.49e+01    5876: 1.91e-04 7065: 2.62e-05  2.06m: 1.29e-02  21c: 5.29e-01
```

The first two lines give the continuum optical depths at various energies. These are the total optical depths, including the correction for stimulated emission, and will be negative if maser action occurs. All opacity sources are included. The labels, and their interpretation, are as follows. COMP is the Thomson scattering optical depth. "H-" is the optical depth at the wavelength where the negative hydrogen ion has its greatest maximum cross section. "R(1300)" is the optical depth due to Rayleigh scattering by H^0 at 1300Å. "$H2^+$" is the optical depth at the dissociation threshold of the molecular hydrogen ion. "Bra" is the optical depth at the wavelength of the Brackett α transition (5-4).

The next line gives total continuous optical depths at the energies of various hydrogen and helium ionization edges and mean line optical depths[3]. These are evaluated at the energies of the Paschen α, Balmer α and β, and Lα lines, and the ionization edges of hydrogen, atomic helium, and the helium ion.

The third line gives optical depths of some He I lines. These are computed with a full model of the He^0 atom (Porter et al., 2005).

```
Old, new H  1 continuum optical depths:
     1 1.13e+05     2 3.68e+03     3 1.69e+03     4 8.24e+02     5 4.03e+02     6 2.12e+02     7 1.24e+02     8 8.47e+01
     9 7.60e+01    10 3.02e+02    11 2.24e+02    12 1.05e+02    13 9.80e+01    14 1.31e+02    15 1.16e+02    16 9.21e+01
    17 7.61e+01    18 6.54e+01    19 5.68e+01    20 4.88e+01    21 4.19e+01    22 3.55e+01    23 3.00e+01    24 2.55e+01
    25 2.17e+01
     1 1.13e+05     2 3.61e+03     3 1.66e+03     4 8.08e+02     5 3.95e+02     6 2.08e+02     7 1.22e+02     8 8.31e+01
     9 7.46e+01    10 2.96e+02    11 2.20e+02    12 1.03e+02    13 9.61e+01    14 1.28e+02    15 1.14e+02    16 9.03e+01
    17 7.46e+01    18 6.41e+01    19 5.57e+01    20 4.78e+01    21 4.11e+01    22 3.48e+01    23 2.95e+01    24 2.50e+01
    25 2.12e+01

 Old, new H  1 line optical depths:
  2- 1 2.59e+09  3- 2 1.58e-01  4- 3 9.14e-08  5- 4 5.27e-08  6- 5-1.66e-08  7- 6-1.39e-07  8- 7-5.70e-07
  9- 8-1.24e-06 10- 9-1.79e-06 11-10-3.40e-06 12-11-4.47e-06 13-12-4.36e-06 14-13-3.91e-06 15-14 9.70e-06 16-15-6.04e-05
 17-16-1.08e-04 18-17-1.88e-04 19-18-3.44e-04 20-19-6.90e-04 21-20 1.37e-02 22-21 2.07e-02 23-22 6.52e-02 24-23 8.91e-02
 25-24 1.18e-01
  2- 1 1.16e+09  3- 2 7.08e-02  4- 3 6.02e-08  5- 4 2.67e-08  6- 5-2.15e-08  7- 6-1.51e-07  8- 7-5.76e-07
  9- 8-1.23e-06 10- 9-1.78e-06 11-10-3.35e-06 12-11-4.41e-06 13-12-4.30e-06 14-13-3.81e-06 15-14 4.83e-06 16-15-5.97e-05
 17-16-1.07e-04 18-17-1.85e-04 19-18-3.39e-04 20-19-6.74e-04 21-20 6.72e-03 22-21 1.01e-02 23-22 3.20e-02 24-23 4.38e-02
 25-24 5.79e-02

 Old, new He 2 continuum optical depths:
     1 4.47e+06     2 1.12e+05     3 4.60e+03     4 3.68e+03     5 2.54e+03     6 1.69e+03     7 1.17e+03     8 8.24e+02
     9 5.77e+02    10 4.03e+02    11 2.88e+02    12 2.12e+02    13 1.61e+02    14 1.24e+02    15 1.01e+02    16 8.47e+01
    17 7.13e+01    18 7.60e+01    19 1.43e+02    20 3.02e+02    21 3.11e+02    22 2.24e+02    23 1.54e+02    24 1.05e+02
    25 8.75e+01
     1 4.38e+06     2 1.13e+05     3 4.52e+03     4 3.61e+03     5 2.50e+03     6 1.66e+03     7 1.15e+03     8 8.08e+02
     9 5.66e+02    10 3.95e+02    11 2.82e+02    12 2.08e+02    13 1.57e+02    14 1.22e+02    15 9.93e+01    16 8.31e+01
    17 7.00e+01    18 7.46e+01    19 1.40e+02    20 2.96e+02    21 3.05e+02    22 2.20e+02    23 1.51e+02    24 1.03e+02
    25 8.58e+01

 Old, new He 2 line optical depths:
  2- 1 7.60e+06  3- 2 6.42e-07  4- 3 2.62e-13  5- 4-1.24e-12  6- 5-5.54e-12  7- 6-1.45e-11  8- 7-2.98e-11
  9- 8-5.02e-11 10- 9-7.50e-11 11-10-9.49e-11 12-11-9.32e-11 13-12-3.54e-11 14-13 2.08e-10 15-14 1.07e-09 16-15-1.24e-09
 17-16-2.30e-09 18-17-3.80e-09 19-18-6.67e-09 20-19-1.30e-08 21-20 2.38e-07 22-21 3.59e-07 23-22 1.20e-06 24-23 1.63e-06
 25-24 2.15e-06
  2- 1 4.03e+06  3- 2 3.21e-07  4- 3 1.31e-13  5- 4-1.23e-12  6- 5-5.53e-12  7- 6-1.44e-11  8- 7-2.97e-11
  9- 8-5.01e-11 10- 9-7.48e-11 11-10-9.47e-11 12-11-9.29e-11 13-12-3.54e-11 14-13 1.04e-10 15-14 5.32e-10 16-15-1.23e-09
 17-16-2.30e-09 18-17-3.80e-09 19-18-6.66e-09 20-19-1.30e-08 21-20 1.18e-07 22-21 1.78e-07 23-22 5.96e-07 24-23 8.09e-07
 25-24 1.07e-06

 Old He Is optical depths:   1 3.86e+07   2 4.04e+03   3 3.94e+03   4 3.80e+03   5 3.80e+03   6 3.80e+03   7 3.67e+03   8 2.16e+03
 New He Is optical depths:   1 3.79e+07   2 3.96e+03   3 3.86e+03   4 3.72e+03   5 3.72e+03   6 3.72e+03   7 3.60e+03   8 2.12e+03
          Old He Is Lines: 2-1 9.19e+11 3-2 6.78e-09
          New He Is Lines: 2-1 4.51e+11 3-2 3.44e-09
```

Hydrogen and helium optical depths in continua and $\alpha(n \rightarrow n-1)$ transitions follow. The first block of lines are the optical depths assumed at the start of the present iteration and the second

[3]Line center optical depths were reported through version C10. Mean line optical depths are now given, although the code works with line center optical depths internally.

block gives the newly computed total optical depths. Negative optical depths indicate maser action. For each of the pairs the first block is the optical depth at thresholds of levels of hydrogen. The optical depths in the $\alpha(n \rightarrow n-1)$ transitions of hydrogen or helium follow.

```
Line Optical Depths: 10830: 3.52e+01  3889: 1.51e+00    5876: 2.11e-08 7065: 2.88e-09  2.06m: 2.86e-05  21c: 5.35e-05
H  1 1215A 5.15e+05 H  1 1025A 8.26e+04 H  1  972A 2.87e+04 H  1  949A 1.35e+04 H  1  937A 7.45e+03 H  1  930A 4.56e+03
H  1  926A 3.00e+03 H  1  923A 2.08e+03 H  1  920A 1.51e+03 H  1  919A 1.12e+03 H  1  918A 8.62e+02 H  1  917A 6.75e+02
H  1  916A 5.39e+02 H  1  915A 4.37e+02 H  1  915A 3.59e+02 H  1  914A 2.99e+02 H  1  914A 2.52e+02 H  1  914A 2.14e+02
H  1  914A 1.83e+02 H  1  913A 1.58e+02 H  1  913A 1.37e+02 H  1  913A 1.20e+02 H  1  913A 1.06e+02 H  1  913A 9.34e+01
--------
```

Line optical depths are not normally printed, but will be if the **print line optical depths** command is entered.

1.10.8 Column densities

```
                                                Log10 Column density (cm^-2)
Htot  : 25.107   HII   : 21.167   HI    : 21.830   H-    : 12.687   H2g   : 24.806   H2*   : 16.421   H2+   : 11.203   HeH+  : 11.485
H3+   : 13.820
CH    : 17.799   CH+   : 12.136   OH    : 14.764   OH+   : 11.763   O2    : 17.909   CO    : 21.489   CO+   : 10.423   H2O   : 17.459
H2O+  : 11.049   O2+   : 11.735   H3O+  : 14.429   CH2+  : 11.869   CH2   : 17.534   HCO+  : 15.394   CH3+  : 13.437   SiH2+ : 11.835
SiH   : 15.523   HOSi+ : 14.069   SiO   : 17.953   SiO+  :  9.222   CH3   : 20.296   CH4   : 20.207   CH4+  : 11.132   CH5+  : 13.562
N2    : 20.644   N2+   : 12.546   NO    : 15.954   NO+   : 12.873   S2    :  4.242   S2+   :  0.565   OCN   : 12.648   OCN+  :  9.954
NH    : 14.634   NH+   :  9.266   NH2   : 16.135   NH2+  :  9.125   NH3   : 16.966   NH3+  : 12.225   NH4+  : 13.243   CN    : 18.325
CN+   :  7.814   HCN   : 18.107   HCN+  :  8.175   HNO   :  8.826   HNO+  : 10.277   HS    : 14.673   HS+   : 13.458   CS    : 19.929
CS+   : 10.371   NO2   : 10.136   NO2+  :  4.356   NS    : 13.418   NS+   : 12.254   SO    : 19.303   SO+   : 14.554   SiN   : 13.857
SiN+  : 10.516   N2O   : 10.072   HCS+  : 15.996   OCS   : 19.077   OCS+  : 14.312   C2    : 20.023   C2+   : 11.133   CCl   : 14.010
ClO   :  2.369   HCl+  : 11.968   HCl   : 17.061   H2Cl+ : 12.002   CCl+  : 12.258   H2CCl+: 10.100   ClO+  : -1.084   HNC   : 18.151
HCNH+ : 14.265   C2H   : 19.590   C2H+  : 10.670   C2H2  : 16.355   C2H2+ : 15.324   C3H   :  4.558   C3H+  : -0.848   C2H3+ : 11.612
C3    :  3.013   C3+   : -6.584   COgrn : 17.793   H2Ogrn: 21.202   OHgrn :  8.957

             1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17

Hydrogen   21.830 21.167 25.107 (H2)                Log10 Column density (cm^-2)
Helium     24.085 20.117 17.105
Carbon     17.950 18.459 17.563 14.609 13.216  3.870
Nitrogen   19.044 16.241 16.933 14.065 11.478  5.692 -1.143
Oxygen     20.608 17.460 17.476 14.327 11.487  6.302  2.306
Neon       20.885 16.857 16.224 13.324 10.890  5.202  0.097
Magnesium  19.584 16.541 15.619 12.650 10.152  4.929  0.953
Silicon    19.701 16.932 15.711 14.515 13.010 10.127  3.809 -0.668
Sulphur    19.036 17.151 16.136 14.583 12.601 11.685 10.014  2.678 -2.437
Chlorine   18.066 14.800 14.129 11.924 10.392  9.305  4.190  1.698 -3.512
Argon      19.584 14.672 15.606 13.401 11.627 10.513  5.326  2.378 -0.441
Iron       19.584 16.655 15.236 15.417 12.498 11.847  9.292  5.178  1.303 -3.214
Exc state    He1* 14.756   C+1[2] 18.248   C[1] 17.606   C[2] 17.569   C[3] 17.067   O[1] 20.607   O[2] 18.042   O[3] 17.426
             Si2* 16.187   C+2[2] 12.885   C+2[3]  8.857   C+2[3] 13.149
```

This lists the column densities (cm^{-2}) of some atoms, ions, and molecules. The first number "Htot" is the total column density of hydrogen in all forms (including atoms, ions, and molecules). The following two numbers are the column densities in H^+ and H^0. The last four numbers are column densities in four ions and molecules (H^-, H_{2g}, H_2^*, H_2^+, H_3^+, and HeH^+). The remaining lines give column densities in various molecules. Molecules with names ending in "grn" are solids that have condensed onto grain surfaces.

The next block gives column densities in atoms and ions of the heavy elements. For hydrogen the last number is the H_2 column density. Column densities within certain excited states of the heavy elements, listed in Table 8.1 on page 78, are also printed. The label gives the element, ionization stage, and level within the ground term. These upper levels are photoexcited by the so-called "level 2 lines". Their pumping will not be included and excited state column densities will not be predicted if the level 2 lines are disabled with the **no level 2 lines** command.

1.10.9 Mean ionization and temperature

```
             1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16

Hydrogen   -3.278 -3.940 -0.000 (H2)                Log10 Mean Ionisation (over radius)
```

```
Helium     -0.000 -3.968 -6.980
Carbon     -3.635 -3.126 -4.021 -6.975 -8.368-17.715
Nitrogen   -1.908 -4.712 -4.019 -6.887 -9.474-15.261-22.096
Oxygen     -1.101 -4.249 -4.234 -7.382-10.222-15.407-19.403
Neon       -0.000 -4.028 -4.662 -7.561 -9.996-15.684-20.788
Magnesium  -0.000 -3.044 -3.966 -6.934 -9.432-14.656-18.631
Silicon    -0.008 -2.778 -3.999 -5.194 -6.700 -9.582-15.900-20.377
Sulphur    -1.071 -2.956 -3.971 -5.524 -7.507 -8.423-10.093-17.429-22.545
Chlorine   -0.041 -3.307 -3.978 -6.184 -7.716 -8.802-13.918-16.410-21.619
Argon      -0.000 -4.912 -3.979 -6.183 -7.957 -9.071-14.259-17.206-20.025
Iron       -0.001 -2.929 -4.348 -4.167 -7.086 -7.737-10.292-14.406-18.282-22.799

              1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16

Hydrogen   -1.292 -0.090 -0.864 (H2)         Log10 Mean Ionisation (over radius*electron density)
Helium     -0.622 -0.119 -3.265
Carbon     -2.105 -0.549 -0.176 -3.188 -4.552-14.000
Nitrogen   -0.770 -0.843 -0.174 -3.101 -5.664-11.546-18.381
Oxygen     -0.813 -0.378 -0.405 -3.646 -6.501-11.692-15.688
Neon       -0.730 -0.171 -0.855 -3.828 -6.272-11.969-17.073
Magnesium  -1.269 -0.741 -0.117 -3.184 -5.702-10.941-14.916
Silicon    -1.764 -0.643 -0.148 -1.382 -2.932 -5.840-12.185-16.662
Sulphur    -2.018 -0.696 -0.122 -1.719 -3.712 -4.627 -6.332-13.714-18.829
Chlorine   -0.856 -0.966 -0.130 -2.390 -3.910 -4.994-10.203-12.695-17.904
Argon      -0.732 -1.160 -0.130 -2.396 -4.146 -5.259-10.544-13.491-16.310
Iron       -1.472 -0.778 -0.478 -0.331 -3.339 -3.971 -6.562-10.691-14.567-19.083
```

The next blocks of output give the log of the mean ionization, averaged over volume, area (if the model is spherical), and over radius. The volume-averaged ionization fraction for ion i of element a is given by

$$\left\langle \frac{n_a^i}{n_a} \right\rangle_{vol} = \frac{\int n_a^i f(r)\, r^2\, dr}{\int n_a f(r)\, r^2\, dr}. \tag{1.15}$$

the area average by

$$\left\langle \frac{n_a^i}{n_a} \right\rangle_{area} = \frac{\int n_a^i f(r)\, r\, dr}{\int n_a f(r)\, r\, dr}. \tag{1.16}$$

and the radius average by

$$\left\langle \frac{n_a^i}{n_a} \right\rangle_{rad} = \frac{\int n_a^i f(r)\, dr}{\int n_a f(r)\, dr}. \tag{1.17}$$

Where n_a is the total gas-phase density and n_a^i is the density in ionization stage i. Similar blocks of information will give the mean ionization weighted by electron density and volume, area, or radius.

```
              1      2      3      4      5      6      7      8      9     10     11     12

Hydrogen   3.127  3.965  1.357 (H2)               Log10 Mean Temperature (over radius)
Helium     1.372  3.961  3.937
Carbon     1.485  3.097  3.957  3.945  3.948  3.972
Nitrogen   1.949  4.004  3.956  3.945  3.951  3.972  3.972
Oxygen     1.586  3.983  3.946  3.956  3.963  3.972  3.972
Neon       1.370  3.968  3.944  3.956  3.961  3.972  3.972
Magnesium  1.357  2.953  3.963  3.951  3.957  3.972  3.972
Silicon    1.354  2.714  3.963  3.945  3.946  3.950  3.972  3.972
Sulphur    1.463  2.867  3.964  3.943  3.946  3.946  3.944  3.972  3.972
Chlorine   1.348  3.198  3.962  3.944  3.947  3.947  3.972  3.972  3.972
Argon      1.370  3.922  3.960  3.945  3.948  3.948  3.972  3.972  3.972
Iron       1.357  2.822  3.984  3.950  3.953  3.947  3.957  3.972  3.972  3.972

              1      2      3      4      5      6      7      8      9     10     11     12

Hydrogen   3.223  3.967  2.109 (H2)    Log10 Mean Temperature (over radius*electron density)
Helium     3.430  3.963  3.959
Carbon     2.234  3.742  3.958  3.945  3.949  3.972
Nitrogen   2.664  4.006  3.958  3.945  3.952  3.972  3.972
Oxygen     2.826  3.985  3.947  3.956  3.963  3.972  3.972
Neon       2.675  3.971  3.944  3.956  3.961  3.972  3.972
Magnesium  2.041  3.498  3.965  3.951  3.957  3.972  3.972
Silicon    1.496  3.474  3.965  3.945  3.946  3.950  3.972  3.972
Sulphur    1.721  3.369  3.966  3.944  3.946  3.946  3.943  3.972  3.972
Chlorine   2.140  3.842  3.964  3.944  3.947  3.948  3.972  3.972  3.972
Argon      2.631  4.016  3.962  3.945  3.949  3.949  3.972  3.972  3.972
Iron       1.803  3.140  3.986  3.952  3.953  3.947  3.956  3.972  3.972  3.972
```

The next blocks give the mean temperature weighted by volume, area, and radius. These are followed by the mean temperature weighted by volume, area, or radius and electron density. In all cases the volume and area averages will only be shown in spherical models.

1.10.10 Convergence statistics

```
---------------Convergence statistics---------------
      1.24 mean iterations/state convergence
      2.67 mean cx acceleration loops/iteration
      1.02 mean iso convergence loops/ion solve
         1 mean steps/chemistry solve
         2 mean step length searches/chemistry step
----------------------------------------------------
```

1.10.11 Final report

```
 Cloudy ends: 196 zones,   1 iteration,  1 caution.  ExecTime(s) 86.97
 [Stop in maincl, Cloudy exited OK]
```

The code ends by listing the number of zones and iterations that were performed and the number of warnings and cautions that occurred. Next comes the elapsed wall-clock time [s]. The last line will say “Cloudy exited OK” if the calculation is successful.

Chapter 2

OBSERVED QUANTITIES

2.1 Overview

This section describes how to convert the quantities actually used or predicted by CLOUDY into commonly observed ones.

2.2 Intensities of various continua

2.2.1 Incident radiation field

The incident radiation field is the light striking the cloud. The main printout printout gives the intensity of the incident radiation field with the label "Inci". The total continuum [units erg s^{-1} or erg cm^{-2} s^{-1}] integrated over all energies is given with this label and a wavelength of 0. The incident radiation field is also evaluated at two wavelengths, 4860 Å and 1215 Å, as λF_λ or νF_ν, [units erg s^{-1} or erg cm^{-2} s^{-1}].

The **save continuum** command will produce a file that contains the entire incident radiation field.

These entries will not be included if the **aperture** command is in effect.

2.2.2 The radiation field at specific wavelengths

The intensity of the diffuse radiation field that is emitted or reflected by the cloud is normally included in the main output in the emission-line printout at a series of energies. These have units λF_λ or νF_ν. See the discussion of the **set nFnu** command in Part 1 for further details. You can easily add more continuum points using the **set nFnu add** command, also described in Part 1.

These entries will not be included if the **aperture** command is in effect.

2.2.3 The radiation field integrated over a range of wavelengths

The emitted radiation field integrated over a series of wavelength bands is included in the main printout. The file `continuum_bands.dat` in the data directory specifies a series of wavelength bands. Table 9.1 on page 98 lists the default bands. The label and wavelength that are printed in

the emission-line output are given in the first two columns of that table. The code will integrate over these bands to find the total radiated energy and report this in the main printout. This is a simple summation with no correction for a filter transmission function. The `continuum_bands.dat` file can be edited to change the number of bands or their detailed properties.

This gives the *total* emission that occurs over the band and includes the incident radiation field and both line and continuum diffuse emission. Under many circumstances the radiation field within a band may be dominated by the incident field. The code can also report the emissivity in any of the emission quantities given in the main printout. For these continuum bands the emissivity will only be the diffuse emission from the cloud and will not include the incident field.

These entries will not be included if the **aperture** command is in effect.

2.3 Emission-Line Equivalent Widths

The equivalent width of an emission or absorption line is the number of Angstroms of the continuum that is equivalent to the energy in the line. It is defined as

$$W_\lambda = \int \frac{F_\lambda^c - F_\lambda^t}{F_\lambda^c} d\lambda \approx -\lambda \frac{F_{line}}{\lambda F_\lambda^c} \quad [\text{units of } \lambda] \tag{2.1}$$

where the fluxes are in the incident continuum (F_λ^c), the total transmitted spectrum (F_λ^t), and the line (F_{line}). By this convention the equivalent width of an emission line is negative.

The code's output can be used to predict a line's equivalent width. The previous section describes several of the radiation fields that are predicted. The code prints the intensity or luminosity of all lines and continua and the intensity of each relative to a normalization line.

The ratio of a line to continuum intensity or luminosity will be the dimensionless ratio $F_{line}/\lambda F_\lambda^c$, part of the last term in equation 2.1. The line equivalent width is this ratio multiplied by the wavelength where the continuum is evaluated. The code reports the incident continuum at several wavelengths with labels "Inci". For instance, you could trick the code into printing the relative intensities of the lines as an equivalent width relative to the continuum flux at 1215 Å by including the commands

```
normalize to "Inci" 1215 scale factor = 1215
```

This has two effects. It gives the intensities relative to the incident continuum at 1215 Å and multiplies this by the continuum wavelength in Angstroms, producing the rightmost ratio in equation 1.

Using this trick, all lines will be given as the equivalent width relative to the continuum at the specified wavelength. It is more common to report equivalent widths relative to the continuum near the line itself. You can do this by scaling the incident SED at the wavelength of the **set nFnu** command by the wavelength you want. You can get this information by using the **save continuum** command to obtain the incident radiation field.

These tricks will allow you to get the equivalent width relative to the incident continuum. You can use other options on the the **set nFnu** command to choose which spectral components contribute to the underlying continuum.

A covering factor will complicate this slightly. (Covering factors are defined in the section *Definitions* in Part I of this document and in Section 5.9 of AGN3.) In the luminosity case partial coverage of the source is taken into account with the **covering factor** command and the luminosities are correct for this coverage. The ratio of line to continuum given in equation 2.1 will represent what is observed. In the intensity case the line intensity is given per unit area of cloud no matter what covering factor is specified. In this second case the ratio in equation 2.1 must be scaled by the covering factor.

2.4 Emission-Line Asymmetries

The inward fraction of the total emission of each line is always predicted by the code. It is not reported by default. Many lines are significantly inwardly beamed and this can lead to emission-line asymmetries if the envelope is expanding. The inward part of the lines will be printed if the **print line inward** command is entered. Note that the effects of this line beaming are very geometry dependent.

2.5 Surface Brightness

CLOUDY will normally predict a line's intensity as $4\pi J$, the intensity radiated into 4π sr by a unit area of cloud, with units erg s^{-1} cm^{-2}. Observations of resolved sources often measure the surface brightness, with units erg s^{-1} cm^{-2} $arcsec^{-2}$ or s^{-1} cm^{-2} sr^{-1}. Be careful! Some workers may report surface brightness with units erg s^{-1} cm^{-2} $arcsec^{-2}$ sr^{-1}. Remove the sr^{-1} before continuing by multiplying by 4π.

To obtain the predicted surface brightness we must divide the intensity $4\pi J$ by the number of square seconds of arc in 4π sr or the number of sr in 4π sr. One radian is $360/2\pi = 57.29578$ degrees, so 1 sr is $(180/\pi)^2 = 3282.806$ $degree^2$. There are $(60\times 60)^2$ square seconds in a square degree, so there are 5.3464×10^{11} square arc seconds in 4π sr. The surface brightness (per square second of arc) is the intensity $4\pi J$ multiplied by the inverse of this, or 1.8704×10^{-12} $arcsec^{-2}$. The surface brightness (per sr) is the intensity $4\pi J$ divided by 4π.

Note that this is only correct for a line that is emitted isotropically, because the code predicts $4\pi J$ while an observer measures I along a particular direction. (The code does predict the fraction of a line that is emitted from the illuminated face of the cloud.) This discussion is only formally correct if $I = J$.

There is a **print line surface brightness** command, described in Section 16.19.19 *Print line surface brightness [arcsec]* of Hazy 1 which will change the intensity into surface brightness units. By default the final units will then be erg s^{-1} cm^{-2} sr^{-1}, but the command has an **arcsec** keyword to specify the surface brightness in erg s^{-1} cm^{-2} $arcsec^{-2}$.

2.6 Flux to luminosity

The luminosity is the intensity of a line multiplied by the total area of the shell. For full coverage this is $4\pi r^2$ where r is the radius of the shell. If the shell only partially covers the continuum source then this should be multiplied by the covering factor.

2.7 Flux at the Earth

If the distance to the object is specified with the **distance** command, and the luminosity case is predicted then the flux observed at the Earth will be predicted if the **print flux at Earth** command also appears.

2.8 Relative hydrogen line intensities

Hydrogen line intensities can be predicted with great precision when Case B applies. Ferguson and Ferland (1997) describe CLOUDY's original hydrogen atom and Ferland et al. (2009) describe its current implementation. It gives good results for all reported lines. The number of reported lines can be increased to go higher in the HI model atom by using the **atom H-like levels** command. This gives better results at the expense of more compute time.

The accuracy of CLOUDY's HI line emissivities is limited by the size of the model hydrogen atom that can be computed on the fly. The definitive calculation for hydrogen recombination is that of Hummer and Storey (1987) and Storey and Hummer (1995), who used a 1000 level atom with all l-levels explicitly considered (that works out to something like a million levels!). The code interpolates on their tables and includes their Case A and Case B predictions within the main printout. The test cases `limit_case*.in` in the test suite compare the code's predictions with their Case B values.

The Hummer and Storey (1987) calculation is for Case B conditions, which assume that many processes are unimportant (see AGN3). Neglected processes include collisional excitation from the ground or first excited states, induced processes where the incident continuum causes the atom to fluoresce, and line transfer in all non-Lyman lines. Case B is often an excellent assumption for galactic nebulae such as planetary nebulae or HII regions. Case B is not valid for gas densities greater than $10^6\,\mathrm{cm}^{-3}$ or when X-rays are present. When any of these processes are important the predictions of CLOUDY's model atom are more realistic than Case B predictions.

2.9 Helium line intensities

The code includes a model of the He^0 atom that is applied all along the helium iso-electronic sequence. The model can have an arbitrarily large number of levels (Bauman et al., 2005; Porter et al., 2005; Porter and Ferland, 2007). The predictions become more exact as the number of levels is increased.

2.10 Line intensities in a dusty cloud

Two sets of line intensities are printed in the main output. The first block of lines, with the title "Intrinsic Intensities", includes all the physics of line formation, including destruction by local background opacities such as grains or photoelectric absorption, but does not include the effects of absorption and scattering of the line from regions away from that were the line forms. This would be the spectrum you would observe after correction for reddening or line of sight extinction.

The second block of emission-line intensities, with the title "Emergent Intensities", includes the effects of absorption and scattering from regions outside those where the lines form. The distinction is important for optical emission from any geometry that has a large dust extinction A_V, for instance, an H^+ layer on the surface of a molecular cloud.

There are two simple limits for dust extinction. If the simulation only includes the ionized region of a photoionized cloud then dust extinction of optical or IR lines will usually be very small. This is because the *total* optical depth across an H^+ layer is usually $\tau \leq 1$ at 912 Å (Baldwin et al. 1991, Bottorff et al. 1998, AGN3 Chapter 2). The dominant opacity is usually the Lyman continuum of hydrogen so the total dust optical depth is $\tau_{dust} \ll 1$. Grain extinction is much smaller in the visual than in the FUV around 912 Å, so the visual extinction will also be small. Extinction is even smaller in the IR due to the much smaller grain opacity there. If the optical emission-line spectrum is reddened it may be caused by layers of dust that reside in neutral gas associated with the source, but far more likely the dust is not associated at all with the object you are modeling and resides in the ISM between the source and the observer.

A second geometry is appropriate for star-forming H II regions like the Orion Nebula. This is a blister H II region on the surface of the Orion Molecular Cloud 1 (Zuckerman 1973; Balick et al. 1974; Baldwin et al. 1991; Ferland 2001b). An idealized geometry is shown in Figure 2.1. Two sets of emission lines are observed, see figure 2 of Castaneda (1988), one radiated directly towards the observer and one reflected off of the background molecular cloud (O'dell et al., 1992). On second and later iterations the code computes the fraction of the line emission that is directed towards the illuminated and shielded faces of the ionized layer. The outward line emission is emitted towards the molecular cloud that will have a large optical depth due to grains. The albedo of the gas-grain mixture is computed and the fraction reflected is passed back towards the illuminated face. The total intensities are roughly half what would be expected were the cloud emitting from both sides since much of the light directed into the molecular cloud is absorbed. Something like 10% of the light striking the molecular cloud will be reflected back to the observer, and so slightly more than 50% of isotropically emitted lines will emerge from the illuminated face. The code uses the albedo of the gas at the wavelength of the line to predict this reflected portion and the full optical depths computed on previous iterations.

Although this option was developed with optical emission from the geometry shown in Figure 2.1 in mind, the treatment is actually quite general. All scattering and absorption opacities are considered, so photoelectric absorption and electron scattering are also included, along with all other opacity sources considered by the code. A closed geometry, described in Hazy 1 Section 2.3.4, *Open vs. closed geometry* can also be computed, in which case all emission will filter out through the outer material, including the PDR and molecular cloud surrounding an H II region. The reflected spectrum is not computed for a closed geometry.

The treatment of the emergent spectrum was heavily modified in C17 to take advantage of the current status of the code. When the reflected component of the spectrum was identified by O'dell et al. (1992) it was not possible to extend a CLOUDY calculation into the PDR and molecular cloud to recover this reflected component. PDR physics was identified as a high priority, leading to the Ph.D Theses of Nick Abel (Abel et al., 2005) and Gargi Shaw (Shaw et al., 2005) more than a decade later.

The emergent spectrum was introduced soon after the O'Dell discovery of the reflected spectrum. The implementation was guided by two considerations. First, all star-forming H II regions lie on the surface of a far larger molecular cloud with large A_V. This is a corollary to the

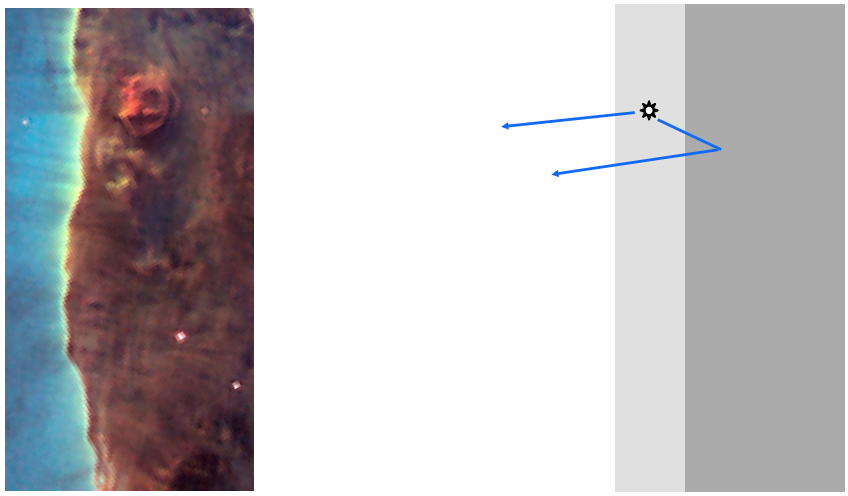

Figure 2.1: The geometry assumed in an open dusty geometry. The panel on the left is part of the HST image of M16, an H^+ layer on the surface of a molecular cloud viewed nearly edge-on. The idealized geometry is shown on the right. The lightly shaded area is the H^+ region, while the darker region to its right in the optically thick molecular cloud. Light produced by an atom in the H^+ region can directly escape from the illuminated face of the cloud. If the atom emits isotropically then roughly half the emission will escape this way. The remaining fraction of the light is emitted towards the molecular cloud where a small part, determined by the albedo, can be reflected back towards the illuminated face.

fact that massive O stars do not live long enough to stray far from their birthplace. Second, CLOUDY could not explicitly compute conditions in the molecular cloud to capture this reflection component.

In versions of CLOUDY between the mid-1990s and C13 the emergent spectrum assumed that the dust optical depth in the outward direction was infinite, a good approximation for a giant molecular cloud. The physics shown in Figure 2.1 could then be captured. This was documented in Hazy1 & Hazy2. The behavior was changed in C17 to only include absorption and scattering by the computed geometry. The scattering component will only be computed if the calculation extends into the molecular cloud. It is not necessary to compute the full molecular cloud. The calculation has to extend to a large optical depth at visual wavelengths. This might be done with, for example, by combining the commands **stop Av 3** and **stop temperature off** to extend the calculation well into the PDR.

These predictions are only reliable once the radiative transfer and line optical depths are well converged. Consider using the **iterate to convergence** command described in Hazy 1 Section 10.7, *Iterate [2 times, to convergence]*.

2.11 Continuum pumping contribution to line intensities

Continuum pumping or fluorescence is included for all lines. The contribution is only explicitly reported if the **print line pump** command is entered. Whether or not this contribution actually adds to the observed line emission depends on the geometry. Continuum pumping increases the line emission if no related continuum absorption occurs. This will be the case if the continuum source is either not observed or not covered by absorbing gas. If absorbing gas covers an observed continuum source then the situation is like the P Cygni problem, and pumping may not increase the net intensity of the line at all (the absorption component will have the same equivalent width as the associated emission). The printed line intensity includes this contribution unless the **no induced processes** command is entered. (The **no induced processes** command has many other effects and so should only be used as a test.)

The output produced by the **save 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.

2.12 Column densities

The column densities of all constituents are printed at the end of the calculation. Column densities within many excited states are also printed. The excited states are identified with a '*'. The table that accompanies the description of the ***cdColm*** command (see Table 8.1 on page 78 above) identifies the various labels.

2.13 A synthetic spectrum

A table of emission-line intensities is part of the normal output. Sometimes a synthetic spectrum, rather than a table, is desired. Very coarse spectra can be generated with the **save continuum** or

save spectrum commands, but a detailed synthetic spectrum is not the main purpose of this output.

It is best to save the emission-line spectrum and then post-process this data using your own software. Then blends of lines can be synthesized at any spectral resolution desired. The spectrum can be save two ways. The main block of emission-line intensities in the final printout can be printed as a single column, which can be sorted by intensity or wavelength (by using options on the **print lines** command in Section 1 of this document). The **save lines, array** command can report the emission lines. Write a small program or script to read these tables and create a final synthesized spectrum.

2.14 Line profiles

The observed line profile can be predicted by integrating the emissivity of the line over the computed structure while taking the local velocity structure into account. The emissivity is obtained with the **save lines emissivity** command, described in Part 1 of this document. This gives the net emission, with units erg cm^{-3} s^{-1}, emitted by a unit volume of gas and emergent from the cloud surface. The total emission is the integral of the emissivity. An integral over radius will give the line intensity $4\pi J$ while an integral over volume will give the luminosity.

The observed profile will depend on the velocity field at each point in the integration. For static models this will be the Voigt function at the local temperature and microturbulence. For a dynamical model it will include bulk motion of the gas.

Chapter 3

LIMITS, ASSUMPTIONS, AND RELIABILITY

3.1 Overview

This section outlines some of the assumptions and limits that define the range of validity of CLOUDY. The code is designed to be autonomous and self-aware, and to check that these limits are not exceeded during a calculation. This self-checking is a central feature of the code since it is designed to be used to compute large grids with thousands of models, where the examination of individual results would not be possible. CLOUDY should print a warning after the last zone results if any aspects of the calculation are in doubt.

3.2 Time steady

CLOUDY does not assume that the gas is in equilibrium. In most cases it does, however, assume that atomic processes occur on timescales that are much faster than other changes in the system, so that atomic rates have had time to become time-steady. It is possible to follow time-dependent conditions or an advective flow.

In practice most calculations assume that the cloud is old enough for atomic processes to have become time steady. The **age** command (described in Part I of this document) should be used to specify the age of the cloud. The code will then confirm that the time-steady assumption is valid by comparing the system's age with a host of rates and timescales, and will generate a warning if the environment is not time-steady.

Various time scales characterize the approach to equilibrium of an ionized gas (see Spitzer, 1962, and Ferland, 1979 for a specific application). Generally, for an ionized gas with nebular temperatures ($T \sim 10^4\,\mathrm{K}$), the longest is the H^+ recombination time scale,

$$T_{rec} = \frac{1}{\alpha_A\left(T_e\right) n_e} = 7.6 t_4^{0.8}\, n_4^{-1} \text{ years} = 0.66 t_4^{0.8}\, n_9^{-1} \text{ hours} \tag{3.1}$$

where t_4 is the temperature in units of $10^4\,\mathrm{K}$, n_9 is the electron density in units of $10^9\,\mathrm{cm}^{-3}$, and case A recombination is assumed (AGN3).

The time scales are far more ponderous in molecular regions. Generally among the longer of the time scales is the time to form H^-, an important pacesetter for H_2 formation in grain-free environments. This time scale is roughly given by

$$T_{molecule} = \frac{1}{\alpha_{rad}\,(T_e)\,n_e} = 0.3\,t_3^{-0.8}\,n_9^{-1}\ \text{years} \tag{3.2}$$

where t_3 is the temperature in units of 10^3 K.

If the age of the cloud is not long enough for atomic processes to become time steady then a time-dependent calculation should be done. If the gas flow is fast enough for advection to add significant terms to the statistical equilibrium equations then a wind calculation should be performed. Commands for these simulations are described in Chapter 14, *DYNAMICAL & TIME-DEPENDENT CALCULATIONS*, in Hazy 1.

3.3 Atomic and molecular database

This section outlines some of the atomic and molecular physics issues that affect the reliability of numerical simulations of nebulae. These uncertainties were extensively discussed in the Lexington Plasma 2000 meeting (ASP Conf series 247, *Spectroscopic challenges of photoionized plasmas,* Gary Ferland & Daniel Savin, editors) and they underscore the importance of atomic and molecular physics for the interpretation of astrophysical spectroscopy.

3.3.1 Collisional processes

By its nature, the electron temperature of a photoionized gas is low compared with the ionization temperature of the mixture of atoms and ions, as defined by the Saha equation (if the two were comparable, the gas would be collisionally ionized). Because of this, the rate coefficients describing collisional effects, such as the production of cooling emission lines, are often dominated by the cross sections near threshold. This is where laboratory experiments are difficult and *ab initio* quantum theory must often be used. As a result, the collision strengths undergo constant revision, towards better and more reliable values.

To cite one extreme example, the collision strength for transitions within the ^3P ground term of Ne^{+4} underwent three revisions between 1984 and 1991, each by a factor of 10, because of theoretical uncertainties in positions of autoionizing states with unknown energies (Lennon and Burke, 1991). The intensities of all emission lines can be affected by major changes in the atomic data for only one line for some conditions. This is because (in this case) the infrared fine structure lines of Ne^{+4} can be important coolants in low-density high-ionization gasses such as planetary nebulae, and changing their cooling rate alters the thermal structure of the entire nebula. Such changes often give even models of time-steady objects such as planetary nebulae certain time-dependent characteristics.

At present, there are fairly reliable calculations of collision strengths and transition probabilities for the majority of the strong optical and ultraviolet lines in moderate ionization nebulae. A series of papers by Oliva and collaborators (see Oliva et al., 1996 and van Hoof et al., 2000) outline observational evidence concerning accuracies in collision strengths of moderate ionization far infrared lines.

Some strong cooling lines of high ionization species do not have accurate collision rates. As an example, few of the "level2" lines included in the code have real collision strengths. Various forms of the "g-bar" approximation are used for those lines that do not have accurate collision rates.

3.3.2 Photoionization cross sections

The photoionization cross-section database has undergone a dramatic improvement with the completion of the Opacity Project (Seaton, 1987) and its fitting with analytic approximations (Verner et al., 1996). These are the photoionization cross sections used by CLOUDY and they should be as accurate as 10%. All inner shell multi-electron processes are included (Kaastra and Mewe, 1993) using distorted wave cross sections (referenced in Verner et al.). This part of the data base is in fairly good shape, although greater accuracy is always desired.

"Fano profiles", due to autoionization resonances, appear as large changes in photoionization cross section that occur over a narrow range of energy, are averaged over, as described by Verner et al. Their positions are not accurately known, and they could make a difference if sharp spectral features occur in the stellar continuum at the position of a resonance. The photoionization rate could be changed dramatically in this case. Experimental data would be needed to upgrade the photoionization data base to include Fano profiles.

3.3.3 Recombination rate coefficients

Recombination from closed shell species is accurately known (Verner and Ferland, 1996) since these are dominated by radiative recombination. Reliable dielectronic recombination coefficients do not now exist for most other stages of ionization. Currently there is no theory that can reproduce the best experiments (Savin et al., 1999). For these, CLOUDY uses the guestimates described in Part I of this document. This is clearly the greatest single gap in the atomic data base today. Savin (2000) shows an example where this uncertainty has a direct impact on cosmological studies.

3.3.4 Charge transfer

The rate coefficients for charge transfer are another uncertainty in the atomic and molecular database. This process is sometimes the dominant neutralization mechanism for singly or doubly ionized heavy elements. At present many charge exchange rate coefficients are the result of Landau-Zenner calculations using semi-empirical potential curves (Kingdon and Ferland, 1996, Kingdon and Ferland, 1999). These are thought to be no more accurate than a factor of three. Even the best quantal calculations are not thought to have an accuracy much better than 50 percent. Unpublished tests suggest that these uncertainties affect some line intensities at the $\sim$20% level, and a few by more than this.

3.4 Continuous opacity

All significant continuous opacity sources are treated for the energy range considered by the code, 3.040×10^{-9} Ryd to 7.354×10^{6} Ryd. These opacity sources include inverse bremsstrahlung,

grains (when present), H^- absorption, electron scattering, the damping wings of strong resonance lines (i.e., Rayleigh scattering), pair production, photoelectric absorption by the ground and excited states of all ions of the lightest 30 elements, and photoabsorption by molecules. This treatment should be adequate as long as the optical depths to electron scattering are not large. CLOUDY is not now designed to simulate Compton-thick regimes. (A warning will be issued after the last zone calculation if the nebula is very optically thick to electron scattering.)

3.5 Temperature range

CLOUDY assumes that the electrons are non-relativistic, which limits it to temperatures below roughly 10^9 K. CLOUDY goes to the Compton temperature of the radiation field to great accuracy in the limit of very high levels of ionization for blackbody radiation fields with temperatures between 2.8 K and 1.001×10^{10} K. There is no formal lower temperature limit to its validity. Note that very cold gas is rarely in steady state, however, because of the very slow collision rates. Similarly, the collision timescales in very hot gas ($T \gg 10^8$ K) are not rapid enough to ensure that the electrons and ions have the same temperature, or that heating - cooling balance has become time steady (Johnson and Quataert, 2007). Electron-ion decoupling is not now included.

The range of validity of the code is approximately from 10 K to 10^9 K. Temperatures outside this range can still be treated, although with greater uncertainty. The code will not permit temperatures below 2.8 K or above 1.001×10^{10} K.

3.6 Density range

There is no formal lower limit to the density that CLOUDY can treat. The set of heavy element fine structure lines, which dominate cooling at low densities, is complete for astrophysically abundant elements, and fine structure line optical depths, continuum pumping, and maser effects are fully treated.

There is no formal high-density limit, although the simulation is less complete at high ($n \cong 10^{10}\,\mathrm{cm}^{-3}$ densities. Line radiative transfer processes are fully treated with either escape or Sobolev approximations (see Kalkofen, 1987 and Avrett and Loeser, 1988) and collisional-radiative ionization processes for excited levels of the heavy elements are treated. All species of H-like and He-like isoelectronic sequences are treated as many-level atoms, including all of the physical processes that allow the approach to LTE (see, for example, Mihalas, 1978). Tests with a hydrogen density of $10^{19}\,\mathrm{cm}^{-3}$ show that the hydrogen and helium atoms and the hydrogen molecules go to LTE at high densities. They go to strict thermodynamic equilibrium when exposed to a true black body. The treatment of Stark broadening for hydrogen lines follows Puetter (1981), so line radiative transfer is treated correctly (in the context of the escape probability formalism) for densities above $\sim 10^{10}\,\mathrm{cm}^{-3}$.

The treatment of the other 28 isoelectronic sequences is presently not as complete as the H and He-like sequences. Three-body recombination is included as a general recombination process, so the treatment of these elements is approximately correct at high densities.

CLOUDY has been tested at densities of $10^{-8}\,\mathrm{cm}^{-3}$ and $10^{19}\,\mathrm{cm}^{-3}$ on 32-bit machines. The numerical (not physical) limit to the density will actually be set by the limits to the range of the

floating point numbers allowed by the machine in use. The physics incorporated in the code imposes no lower limit to the density. The physical high-density limit is roughly $10^{15}\,\mathrm{cm}^{-3}$, and is set by the approximate treatment of three-body recombination - collisional ionization for the heavy elements.

3.7 Radiative transfer

Several tests presented in the test suite show that the continuum transfer methods are in excellent agreement with known exact results.

Line intensities are predicted with stellar atmosphere conditions in mind. Radiative transfer effects, including continuum pumping and possible maser emission, are treated. Nebular approximations, such as the approximation that all atoms are in the ground state, are not made. Collisional effects, including excitation and de-excitation, continuum fluorescence, recombination, etc, are all included as general line excitation mechanisms. The treatment of level populations is designed to go to LTE in the high particle or photon density cases.

The transfer of subordinate lines, those where both upper and lower level of the transition occur in excited state, of the H-like and He-like iso sequences at high ($n \gg 10^{10}\,\mathrm{cm}^{-3}$) densities is a concern. Resonance lines should be fine.

3.8 Reliability

Several issues affect the general question of the reliability of the code. The first is the effects of the bugs that surely must exist in a code the size of CLOUDY. I have seldom found bugs in sections of the code older than roughly two to three years. Younger sections of the code sometimes contain bugs that only manifest themselves in exceptional situations. The issue of reliability in the face of complexity will increasingly be the single major problem limiting the development of large-scale numerical simulations (Ferland, 2001a). New methods of writing code will have to be developed if we are to take full advantage of the power of future machines. Machines are getting faster more quickly than people are getting smarter.

The second issue is the validity of the numerical methods used to simulate conditions in the plasma. Fundamental uncertainties arise for cases where the density is high ($n \gg 10^{10}\,\mathrm{cm}^{-3}$). The line radiative transfer techniques used by CLOUDY are approximate (see the discussion by Avrett and Loeser, 1988). Unfortunately, no definitive calculation now exists for the complete non-LTE equilibrium and line emission for an intermediate density $\sim 10^{13}\,\mathrm{cm}^{-3}$ cloud. For less extreme conditions ($n < 10^{10}\,\mathrm{cm}^{-3}$) nebular approximations are valid.

Test cases that are designed to exercise the code in well-posed limits and for certain standard nebulae are in the test suite. The code is well behaved and agrees with predictions of similar codes in these limits. The discussion presented in Ferland (1995) and Péquignot et al. (2001) suggests that 10% accuracy can be reached for the intensities of the stronger lines.

The uncertainties can probably best be judged by looking at both the dispersions among the various photoionization calculations presented in Ferland (1995) and Péquignot et al. (2001), and by the changes in the test suite. Much of the dispersion is due to improvements in the atomic database.

There can be little better way to close a discussion of reliability than to quote the warning included in the description by (Kurucz, 1970, see page xiii) of ATLAS5, a code more than an order of magnitude smaller than CLOUDY:

> ***WARNING***
>
> "There is no way to guarantee that ATLAS5 does not contain errors. In fact, it is almost certain that it does, since the code is so long... We also point out that the computation of a model atmosphere should be considered a physical experiment. The program may not be able to calculate a model for conditions that do not occur in real stars or for conditions that violate the initial assumptions on which the program is based."

3.9 The future

The eventual goal is for CLOUDY to give reliable results for all extremes of conditions between and including the intergalactic medium and stellar atmospheres. I estimate that the code is now well over halfway complete.

Current work centers on taking advantage of parallel machines. Once finished, we will be able to use this additional computational power to improve the treatment of hydrodynamics, line radiative transfer, and higher-order dimensionality.

Chapter 4

THE CONTINUUM

4.1 Overview

Under most circumstances the radiation field produced by the central object is the only source of heat and ionization. This section describes how this continuum is treated.

4.2 Attenuation of the incident continuum

In an ***open geometry*** scattering attenuates the incident continuum as

$$I = I_o(1 + 0.5\, d\tau_{scat})^{-1}. \tag{4.1}$$

Scattering does not affect the continuum in a ***closed geometry***. Absorption attenuates the incident continuum as

$$I = I_o \exp(-d\tau_{abs}). \tag{4.2}$$

for both geometries.

4.3 Recombination equilibrium

4.3.1 On-the-spot approximation

A modified version of the "on-the-spot" (OTS) approximation is used in the treatment of sources of diffuse ionizing radiation when the **diffuse OTS** command is used. Were no other opacity sources present, then, for a closed geometry that is optically thick in the Lyman continuum, all recombinations of hydrogen or helium to the ground state would produce ionizing photons. Other atoms of the recombined species would quickly absorb these. In this case OTS is an excellent approximation (van Blerkom and Hummer, 1967; Baessgen et al., 1988). However, other opacity sources are present, and these compete in absorbing protons produced by recombinations, making the recombination process more efficient than the OTS approximation would suggest.

The recombination coefficients are modified by the presence of all other opacity sources, such as grains, free-free or H^- absorption, and the heavy element opacities, in the following manner. The net effective recombination rate coefficient ($cm^3\ s^{-1}$) to level n, $\hat{\alpha}(T_e, n)$, is written in terms

of the spontaneous radiative recombination rate coefficient $\alpha(T_e,n)$ and the opacities (cm^{-1}) κ_n and κ_o for the level n and other opacity sources respectively, as

$$\hat{\alpha}(T_e,n) = \alpha(T_e,n)\left\{P_c(n) + [1-P_c(n)]\left(\frac{\kappa_o}{\kappa_o+\kappa_n}\right)\right\}, \tag{4.3}$$

where $P_c(n)$ is the continuum escape probability. In general, $P_c(n)$ varies between 0 and 0.5 for an optically thick open geometry (see, for example Davidson, 1977), $P_c \sim 1$ if the gas is optically thin, and $P_c \sim 0$ for ground states if the gas is optically thick and the geometry is closed. All computed opacity sources are included in κ_o.

These recombination continua produce a flux of local on-the-spot photons, φ_{OTS} ($\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$). The OTS photoabsorption rate Γ_{OTS} (s^{-1}), used to determine the ionization or heating rate for the gas or grain constituents, is then $\Gamma_{OTS} = \alpha_\nu \varphi_{OTS}$ where α_ν is the absorption cross section at frequency ν. The OTS flux is related to the spontaneous recombination rate coefficient by

$$\varphi_{OTS} = \alpha(T_e,n)\; n_e\, n_{ion}\left[\frac{1-P_c(\tau)}{\kappa_o+\kappa_n}\right]\;\mathrm{cm}^{-2}\;\mathrm{s}^{-1} \tag{4.4}$$

where n_{ion} is the density of the ion. These are stored in the vectors *otscon* and *otslin*, which map one-to-one onto the vectors *flux* and *anu*.

4.3.2 Outward only approximation

A composite "outward-only" (Tarter, 1967) –"on-the-spot" approximation is used in the treatment of sources of diffuse ionizing radiation when the **diffuse outward** command is used. This is the default assumption. The escaping radiation is then propagated in the outward direction (all for the spherical case, and half for an open geometry).

4.4 Continuous opacities

The cloud is divided into a large number of concentric shells (zones) and the attenuated and diffuse continua and physical conditions are then determined within each.

The main opacity sources in the ultraviolet continuum are generally photoelectric and free-free (inverse bremsstrahlung) absorption, grain opacity, electron scattering (of both bound and free electrons), and the damping wings of Lyman lines (Rayleigh scattering). The main reemission mechanisms are generally free-free (bremsstrahlung), grain emission, free-bound, and two-photon emission. Grains are not present by default but can be added as an option. Continuous absorption and reemission by all ground states, and many excited states, of all ionization stages of the 30 elements in the calculation are explicitly included. Great care is taken to ensure that each absorption mechanism is balanced by a reemission process, and vice versa, so that energy balance in the strict thermodynamic equilibrium limit can be achieved.

4.4.1 Total opacity arrays

Total absorption opacities (cm^{-1}) are storied in the vector *opac*. Total scattering opacities (cm^{-1}) are stored in *scatop*. The opacities are evaluated in routine *ConvIonizeOpacityDo* and are within the *opac* structure (defined in `opacity.h`).

4.4.2 Cross-section array

Storage. The cross sections per particle (cm^2) for individual species (atoms, ions, molecules, etc) are stored within the array *OpacStack*, a stack array with a single dimension. These cross sections are evaluated when the code is initialized in routine *OpacityCreateAll*.

Array indices. Each species has an associated array index that defines the offset between the origin of *OpacStack*, the frequency array *anu*, and the opacity at the threshold. If this offset has the name *ioff*, for instance, then the cross section at threshold will be given by array element *OpacStack[ioff]*. If *ip* is the index to the threshold energy within *anu*, then the array index to the cross section at energy i will be $i - ip + ioff$.

Individual cross-sections. The function *csphot* returns the cross section at a specific frequency for any species. It has three arguments, 1) the pointer to the frequency in *anu* where the cross section is to be evaluated, 2) the pointer to the threshold for the species, and 3) the *ioff* offset described above. All are integer variables.

4.4.3 Photoionization rates

Photoionization rates (units s^{-1}) can be computed by several functions. Which is used at a particular time is determined by circumstances.

GammaK This computes the photoionization rate with allowance for an arbitrary fluorescence yield. This routine is a major pacesetter for the code since it is used to evaluate the continuum rates in the majority of the cases. The photoionization rate is given by

$$\Gamma_n = 4\pi \int_{\nu_o}^{\infty} \frac{J_\nu}{h\nu}\, \alpha_\nu \, d\nu \quad [s^{-1}]. \tag{4.5}$$

where α_ν is the photoionization cross section [cm^{-2}]. The routine has three integer arguments, the *anu* pointers to the lower and upper energies and the offset to the opacity array *ioff* (described above).

GammaPrt This is a special version of *GammaK* that writes the step by step results of the integration on any open file. The output lists the product of the photon flux and the cross section, the photon flux, and the opacity.

GammaBn This is a special version of *GammaK* that is used when the correction for stimulated emission or induced recombination is important. The photoionization rate is given by

$$\Gamma_n = 4\pi \int_{\nu_o}^{\infty} \frac{J_\nu}{h\nu}\, \alpha_\nu \, d\nu \quad [s^{-1}] \tag{4.6}$$

and the rate for induced recombination and its associated cooling is computed as

$$\alpha\,(ind) = P_n^* 4\pi \int_{\nu_o}^{\infty} \frac{J_\nu}{h\nu}\, \alpha_\nu \exp\left(-h\nu/kT\right)\, d\nu \quad [cm^3\ s^{-1}]. \tag{4.7}$$

where P^* is the LTE population.

GammaPrtRate will print photo rates for all shells of an ion and element. It is called with three arguments, a file handle, followed by the ionization stage and element number on the C scale (0 for H or atoms, etc).

4.4.4 Attenuation within the zone

A correction must be made to account for the attenuation of the continuum across the zone (Netzer and Ferland, 1984). Assuming that the continuum varies across the zone as

$$\frac{I(\nu,\delta r)}{I_o(\nu)} = \exp\left(-\kappa(\nu)\, f(r)\, \delta r\right) \tag{4.8}$$

then the intensity averaged over a zone with thickness δr is

$$\left\langle \frac{I(\nu,\delta r)}{I_o(\nu)} \right\rangle = \frac{1-\exp\left(-\kappa(\nu)\, f(r)\, \delta r\right)}{\kappa(\nu)\, f(r)\, \delta r} \tag{4.9}$$

where $\kappa(\nu)$ is the absorption opacity and $f(r)$ is the filling factor. The coefficients giving this ratio as a function of energy are stored in the vector *tmn*, and are evaluated in routine *radinc*. The continuum stored in *flux* is multiplied by these factors in the same subroutine.

4.4.5 Rayleigh scattering

Clouds with neutral hydrogen column densities greater than $10^{23}\,\mathrm{cm}^{-2}$ are optically thick to Rayleigh scattering at wavelengths near Lα, and this process is a major scattering opacity source at short wavelengths for grain-free environments.

Rayleigh scattering cross sections given by Gavrila (1967) are used, joined with expressions for the radiative damping wings of Lyman lines (Mihalas, 1978). For wavelengths longward of 1410 Å a power-law fit to Gavrila's quantal calculations is used;

$$\sigma_{Ray} = 8.41\times10^{-25}\varepsilon^4 + 3.37\times10^{-24}\varepsilon^6 + 4.71\times10^{-22}\varepsilon^{14} \quad \mathrm{cm}^2 \tag{4.10}$$

where $\varepsilon \equiv /cR_\infty$ is the photon energy in Rydbergs. This fit is accurate to typically a percent, with occasional errors as large as 4 percent.

For wavelengths between 1410 Å and the Lyman limit, radiative broadening of the Lyman lines is assumed (Mihalas, 1978);

$$\sigma_{Ray} = \sum_{i=2}^{4} \left(\frac{q_e^2\, f_{1,i}}{m_e c}\right) \frac{\Gamma/4\pi}{\left(\nu-\nu_{1,i}\right)^2} \quad \mathrm{cm}^2 \tag{4.11}$$

where Γ is the reciprocal lifetime of the upper level i and the sum is over the first four Lyman lines. This expression gives cross sections in excellent agreement with Gavrila (1967) for these wavelengths.

4.4.6 Free-free opacity

The main opacity source in the infrared-radio spectral region for many conditions is free-free opacity with a cross section given by

$$\alpha_\nu(ff) = 3.69\times10^8\, \bar{g}_{III}(\nu,T)\; f(r)\; \nu^{-3}\, T^{-1/2} \left\{1-\exp\left(-h\nu/kT\right)\right\} \sum_A \sum_z z^2\, n_A^{+z} \quad [\mathrm{cm}^{-2}] \tag{4.12}$$

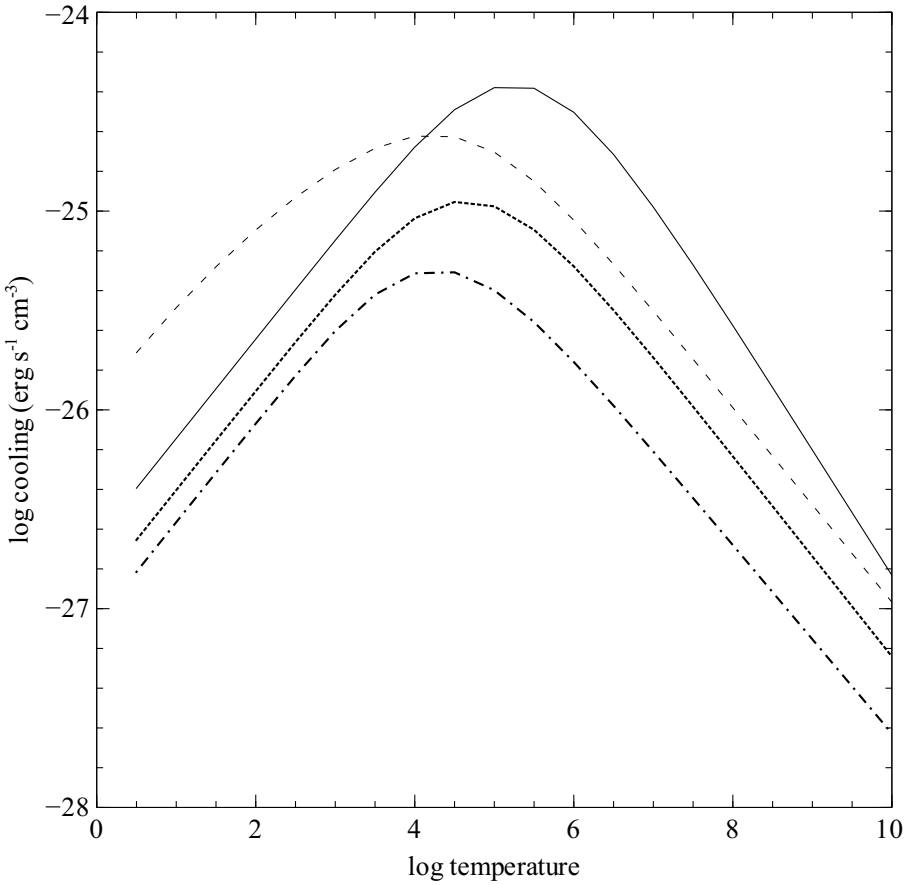

Figure 4.1: Thermally averaged free-free gaunt factor. The gaunt factor is shown as a function of photon energy and temperature.

(see, for example, Mihalas, 1978). The sum is over all ions n^{+z} of element A and over all elements. The temperature averaged gaunt factor $\bar{g}_{III}(\nu,T)$ is taken from Hummer (1988) (see also Karzas and Latter, 1961) and are evaluated in routine *gffsub* that was originally written by D. Hummer.

This routine did not extend to energies that could be treated by asymptotic expansions of the gaunt factor. *gffsub* was modified by J. Ferguson to extend over the full temperature and energy range considered by CLOUDY, and later extensively rewritten by Ryan Porter. Figure 4.1 shows the gaunt factors as functions of photon energy and temperature.

4.4.7 Bound-free opacity

Continuum optical depths for photoabsorption from level l are given by

$$d\tau_l(\nu) = \alpha_\nu(n)\ n_l\ [1-\exp(-h\nu/kT)/b_l]\ f(r)\ \delta r \tag{4.13}$$

where b_l is the departure coefficient for level l and α_ν is the absorption cross section [cm^{-2}].

4.4.8 Plasma frequency

The plasma frequency, the energy where the index of refraction of an ionized medium goes to zero, is given by

$$\nu_{pl} = \left(\frac{n_e q_e^2}{\pi m_e} \right)^{1/2} = 8.978 \times 10^3 \, n_e^{1/2} \, s^{-1} = 2.729 \times 10^{-12} \, n_e^{1/2} \, \mathrm{Ryd} \tag{4.14}$$

An ionized gas will reflect the incident continuum for energies smaller than this. This shielding becomes important for the energy range considered by CLOUDY for electron densities greater than $\sim 10^7 \mathrm{cm}^{-3}$. For higher densities this process is treated by setting the intensity of the incident continuum to zero for energies below the plasma frequency, adding this portion of the incident continuum to the reflected continuum, and not allowing emission or absorption for any processes that occur below the plasma frequency.

4.4.9 Pressure lowering of ionization potential

The electric field of nearby charges in the continuum acts to lower the ionization potential. The amount by which it is lowered is determined by the electron density. Ryan Porter extended the code to consider all species treated with the iso-electronic model atoms.

4.5 The frequency mesh

The energy interval 3.040×10^{-9} Ryd – 7.354×10^6 Ryd is divided into a number of sections using the contents of the file `continuum_mesh.ini`. Each of these sections has an associated mesh resolution r, and is filled with a large number of frequency cells with nearly exponentially increasing widths.

4.5.1 Frequency mesh logic

To define the frequency mesh, the code will first set up an array of edge frequencies ν^{edge} that define the lower and upper limit of each frequency cell. Assuming we want to set up the edges in a section starting at energy ν_0 and ending at ν_1, the first step is to determine how many frequency cells n_{bin} we will generate in that section:

$$n_{\mathrm{bin}} = \left\lceil \frac{\ln(\nu_1/\nu_0)}{r} \right\rceil . \tag{4.15}$$

From this we can calculate the frequency step size ν_{s}:

$$\nu_{\mathrm{s}} = \exp \left[\frac{\ln(\nu_1/\nu_0)}{n_{\mathrm{bin}}} \right] . \tag{4.16}$$

Finally, the frequency of edge number i is defined simply by:

$$\nu_i^{\mathrm{edge}} = \nu_0 \, \nu_{\mathrm{s}}^i \tag{4.17}$$

for $i \in [0, n_{\mathrm{bin}}]$. Once the edges are defined, we can simply define the center of each frequency cell as the exact midpoint between the two edges, and the width as the difference between the two edge energies.

4.5.2 Routines defining the frequency mesh

Several routines can be used to obtain properties of the frequency mesh, all returning values in Rydberg. The function *anu(i)* gives the energy of the center of frequency cell number *i*. The functions *anumin(i)* and *anumax(i)* give the lower and upper frequency limit of cell number *i*, respectively. The routine *widflx(i)* gives the width of cell number *i*. There are also routines to obtain simple mathematical functions of the center frequency, such as the square, the cube, the square root, or the logarithm. The data used by these routines are set up in the routine *t_mesh::p_SetupMesh*.

4.5.3 Changing the resolution of the mesh

The file `continuum_mesh.ini` contains ordered pairs of continuum energies and resolving powers (defined as $1/r$) that are read by *t_mesh::p_ReadResolution* to set the frequency mesh. Change the contents of `continuum_mesh.ini` to change the resolution of the continuum mesh. The file explains how to do this.

Alternatvely, you can also use the command **set continuum resolution** that will apply a uniform multiplicative factor to the resolution in each section defined in `continuum_mesh.ini`. This command is explained in Section 19.13.9 in Hazy 1.

If the energy resolving power is increased then the code will require more mesh points to cover the full continuum and will run more slowly, but the predicted continuum will have greater detail.

4.6 Continuum generation

The continuum is generated by the function *ffun*. *ffun* has a single argument, the energy in Rydbergs, and it returns the number of photons per unit area, time, and Rydberg, at that energy. *ffun* sums over all the specified continua and applies the appropriate normalization factors. Another function, *ffun1*, evaluates each individual continuum, and is normally called only by *ffun*.

The units, and their conversion to other measures of the continuum, are given below. The photon flux density is:

$$\varphi_\nu(\nu) = \mathrm{ffun}(\nu) \quad [\mathrm{photons\,cm^{-2}\,s^{-1}\,Ryd^{-1}}]. \tag{4.18}$$

This is stored in the photon array:

$$flux(\nu_i) = \varphi_\nu(\nu)\,\delta\nu_i = \mathrm{ffun}(\nu_i) \times widflx(\nu) \quad [\mathrm{photons\,cm^{-2}\,s^{-1}}] \tag{4.19}$$

where *widflx* is an array containing the width of each continuum bin. Finally, the energy flux density is given by

$$f_\nu(\nu) = \mathrm{ffun}(\nu)\,h\left(\frac{\nu}{\nu_{912}}\right) \quad [\mathrm{erg\,cm^{-2}\,s^{-1}\,Hz^{-1}}] \tag{4.20}$$

and

$$\nu f_\nu(\nu) = \mathrm{ffun}(\nu)\,h\left(\frac{\nu}{\nu_{912}}\right)\nu_{912}\,h\nu_{Ryd} \quad [\mathrm{erg\,cm^{-2}\,s^{-1}}]. \tag{4.21}$$

4.7 Energy units; the Rydberg

Continuum energies are usually given in Rydbergs. The energy of level n of a hydrogenic atom is given by

$$E_n = -\frac{\mathscr{R}_{\rm H}}{n^2}, n = 1,2,3,\ldots, \quad [\text{units of } \mathscr{R}_{\rm H}] \tag{4.22}$$

where the Rydberg energy is given by

$$\mathscr{R} = \frac{\mu q_e^4}{2\hbar^2} = \frac{\mu}{m_e}\mathscr{R}_\infty \tag{4.23}$$

and the reduced mass of the orbiting electron μ is related to the electron and nuclear mass m_e and m_{nuc} by

$$\mu = \frac{m_e m_{nuc}}{m_e + m_{nuc}} = \frac{m_e}{1 + m_e/m_{nuc}} \quad [\text{g}], \tag{4.24}$$

(Friedrich, 1998). Note that as $m_{nuc} \rightarrow \infty$, $\mu \rightarrow m_e$. This Rydberg energy $\mathscr{R}_{\rm H}$ is smaller than the energy for an infinite mass nucleus $\mathscr{R}_\infty$ by the ratio μ/m_e. Using the 1998 CODATA revision of the fundamental constants (see Cohen and Taylor, 1987; Mohr and Taylor, 2000) the infinite mass Rydberg energy is given by

$$\mathscr{R}_\infty = \frac{m_e q_e^4}{2\hbar^2} = 13.605698 [\text{eV}] \tag{4.25}$$

and

$$\begin{array}{c} \mathscr{R}_\infty / (2\pi\hbar c) = 109737.315686 \text{ cm}^{-1} \\ \mathscr{R}_\infty / (2\pi\hbar) = 3.28984196038 \times 10^{15} \text{ Hz} \\ (2\pi\hbar c) / \mathscr{R}_\infty = 91.126732 \text{ nm} \end{array} . \tag{4.26}$$

The ionization potential of hydrogen $\mathscr{R}_{\rm H}$ is μ/m_e or ~ 0.99946 times smaller than $\mathscr{R}_\infty$. [1] We have

$$\begin{array}{c} \mathscr{R}_{\rm H} = 13.59842 \text{ eV} \\ \mathscr{R}_{\rm H} = 2.179872 \times 10^{-11} \text{ erg} \\ (2\pi\hbar) / \mathscr{R}_{\rm H} = 91.176430 \text{ n}m \\ \mathscr{R}_{\rm H} = 109677.576 \text{ c}m^{-1} \end{array} \tag{4.27}$$

The difference between $\mathscr{R}_{\rm H}$ and $\mathscr{R}_\infty$ is significant since it enters as the third power in the photon phase-space conversion factor $2h\nu^3/c^2$.

The Bohr radius is for an infinite mass nucleus is given by

$$\begin{array}{l} a_o = \hbar^2 / \left(m_e q_e^2\right) = 0.5291772083 \times 10^{-8} \\ a = a_o/\mu \end{array} \quad [\text{cm}]. \tag{4.28}$$

In the "atomic units" system of measuring quantities lengths are given in terms of the Bohr radius and energies in "Hartree" units. One Hartree is twice the Rydberg energy.

[1] $\mathscr{R}_{\rm H}$ was the Rydberg unit used by CLOUDY before 1988.

Chapter 5

LINE ATOMIC PARAMETERS

5.1 Overview

Many atomic physics quantities describe how matter and light interact. This section goes over these quantities and how they are related to one another. The inter-relations between these quantities are described in most spectroscopy texts, at about the same depth as is given below. Hilborn (1982) gives a far more formal description, often tracing quantities back to basic E&M concepts. Highly recommended.

5.2 Spectroscopic notation

A great deal of confusion exists over the difference between the designation of a spectrum and an ion. "Atom II" denotes a spectrum, a collection of photons, while "Atom$^+$" denotes a baryon, the element "Atom" with a single electron removed.

Much of the notation in today's atomic physics was developed in the second half of the 19th century. Physicists noticed that the spectrum of a gas would change dramatically when it was heated to high temperatures. They did not understand the reason why this happened, the electron had not yet been discovered, but they developed the notation that "Atom I" was the normal spectrum, this spectrum changed to "Atom II" when the gas was heated, and became the "Atom III" spectrum if heated still further. The "Atom II" spectrum was often called the "enhanced" spectrum of Atom. This is the reason why, in classical novae, the appearance of broad absorption lines of singly ionized species is called the "diffuse enhanced phase".

The electron was discovered well after this notation had been developed. By the early 20th century it was understood that the "I" spectrum was produced by the atom, Atom^0. At high temperatures the first ion, Atom$^+$, formed and produced the "Atom II" spectrum.

During the first half of the 20th century astrophysicists mainly studied stellar absorption lines. This led to the commonly-used notation that the "Atom II" spectrum, for instance, measured Atom$^+$. It is unambiguously true that the equivalent width of an Atom II absorption line is proportional to the column density of Atom$^+$. However there is an ambiguity in emission lines. The Lα H I line can be produced by impact excitation of H^0 or by recombination of H$^+$. In both cases the line is an H I line, but H I is produced by either H^0 or H$^+$, depending on details.

To be unambiguously correct you should refer to Atom I or Atom II when discussing the

spectrum. When discussing a column density or particle density you should refer to the ion, as in $Atom^0$ or $Atom^+$. It is not correct to refer to the column density of H I. The Lα H I emission line measures the column density of either H^0 or H^+, depending on whether the line forms by impact excitation or recombination. The notation is not ambiguous in absorption lines, which is probably why we have such confusion today. Be unambiguous and correct - use the right notation!

5.3 Line absorption

5.3.1 Line optical depths

The optical depth for a transition $u-l$, where u and l are the upper and lower levels, is given by

$$d\tau_{l,u} = \alpha_\nu \left(n_l - n_u g_l/g_u\right)\ f(r)\, dr \text{ [Napier]}. \tag{5.1}$$

Here $f(r)$ is the filling factor and α_ν is the atomic absorption cross section [cm^2].

The term in parenthesis is the population [cm^{-3}] of the lower level, with a correction for stimulated emission. This term is the only place where stimulated emission enters in the radiative balance equations (Elitzur et al., 1983).

5.3.2 Oscillator strengths

The oscillator strength f is a dimensionless number of order unity that can be thought of as a correction factor to make the expression for a classical oscillator agree with the quantum mechanical value. Sections below relate the oscillator strength to other line parameters such as the absorption coefficient and the transition probability. The absorption (f_{abs}, called $f_{l,u}$ here) and emission (f_{em}, called $f_{u,l}$) oscillator strengths are related by

$$g_l f_{l,u} = -g_u f_{u,l} \tag{5.2}$$

where the g's are the statistical weights. This product is symmetric, neglecting sign, and the code tries to use gf's throughout. The convention is that emission lines have negative oscillator strength.

5.3.3 Absorption cross section

The absorption cross section [cm^2] for a line is related to the dimensionless absorption oscillator strength f_{lu} or f_{abs} by

$$\begin{aligned} \alpha_\nu(x) &= \frac{\pi^{1/2} q_e^2 \lambda\, f_{l,u}}{m_e c u_{\rm Dop}} \varphi_\nu(x) \\ &= 0.014974 f_{l,u} \frac{\lambda_{\rm cm}}{u_{\rm Dop}} \varphi_\nu(x) = 1.4974\times 10^{-6} f_{l,u} \lambda_{\mu{\rm m}} \frac{\varphi_\nu(x)}{u_{\rm Dop}} \end{aligned} \quad [{\rm cm}^2] \tag{5.3}$$

with the relative line displacement given by

$$x \equiv \frac{\nu - \nu_o}{\Delta\nu_{Dop}}, \tag{5.4}$$

$\varphi_\nu(x)$ is the Voigt function, and $u_{\rm Dop}$ is the Doppler velocity width (cm s^{-1}), the point where the line profile falls to 1/e of its peak. With this definition of the relative line displacement, the line profile due to thermal motions alone is $\exp(-x^2)$. The constant part of equation 5.3 (i.e., everything except the rightmost term) is evaluated in routine *abscf*.

The Doppler width for thermal broadening of an atom with atomic mass A is

$$u_{Dop} = \left(\frac{2kT}{m}\right)^{1/2} [\mathrm{cm\,s^{-1}}] = 12.85 \left(\frac{T}{10^4 A}\right)^{1/2} [\mathrm{km\,s^{-1}}] \tag{5.5}$$

(equation 9-35 of Mihalas (1970)).

5.4 The line profile function

5.4.1 Velocities in a thermal distribution

The distribution function for a Maxwellian velocity distribution is given by

$$\frac{n(u)\,du}{n} = \frac{1}{\pi^{3/2}} \exp\left[-u^2 m_A/2kT\right] \left(\frac{m}{2kT}\right)^{3/2} 4\pi u^2\,du \quad [\mathrm{cm\ s^{-1}}] \tag{5.6}$$

(Novotny, 1973; p 122). There are three mean speeds in a thermal velocity distribution. The ***most probable speed*** is the peak of the velocity distribution, with a value

$$u^2_{mean} = 2kT/m_A \quad [\mathrm{cm^2\ s^{-2}}]. \tag{5.7}$$

This is found by setting the derivative of the distribution function to zero (Novotny, 1973, p 122). The velocity distribution function can be expressed in terms of the ***mean speed*** as

$$\frac{n(u)\,du}{n} = \frac{1}{\pi^{3/2}} \exp\left[-u^2/u^2_{mean}\right] \frac{4\pi u^2}{u^3_{mean}}\,du \quad [\mathrm{cm\ s^{-1}}]. \tag{5.8}$$

The ***average speed*** is obtained by averaging over this function and is given by

$$u^2_{average} = 8kT/\pi m_A \quad [\mathrm{cm^2\ s^{-2}}]. \tag{5.9}$$

The ***thermal Doppler velocity width*** is the velocity averaged over the projected line of sight, given by (Novotny, 1973; p 204)

$$u^2_{th} = 2kT/m_A \quad [\mathrm{cm^2\ s^{-2}}]. \tag{5.10}$$

This is the distance from line center where the line profile falls to e^{-1} of its central value. So it turns out that the most probable speed is equal to the Doppler velocity width.

The ***velocity dispersion*** σ is

$$\sigma = u/\sqrt{2} \quad [\mathrm{cm\ s^{-1}}] \tag{5.11}$$

and appears in the Gaussian profile function as

$$\varphi(\delta u) = \exp\left(-\delta u^2/2\sigma^2\right). \tag{5.12}$$

5.4.2 Micro vs macro turbulence

Micro-turbulence (hereafter, just turbulence) is due to any additional motions that occur over scales that are smaller than a photon mean free path. Micro-turbulence changes the line transfer since the line opacity is distributed over a broader range of velocities. Macro-turbulence is due to motion that occurs over such large scale lengths that they not change the optical depth through the emitting region. An example might be cloud orbital motions. The transfer within a cloud is not changed by its bulk motion and so would be considered macro-turbulence.

5.4.3 Line Widths

If a non-thermal micro-turbulent component of motions is present then equation 5.3, the total Doppler velocity width [cm s^{-1}] including turbulence, is given by

$$u_{tot}^2 = 2kT/m_A + u_{turb}^2 \quad [\mathrm{cm^2\ s^{-2}}] \tag{5.13}$$

as determined by the local kinetic temperature T. Within the code the micro-turbulent velocity u_{turb} is assumed to be zero unless it is reset with the **turbulence** command.[1]

In *GetDopplerWidth* the Doppler velocity width is evaluated as

$$u_{Dop} = \sqrt{2kT/m_A + u_{turb}^2} = \sqrt{1.651\times10^8\, T/m_{AMU} + u_{turb}^2} \quad [\mathrm{cm\,s^{-1}}]. \tag{5.14}$$

The atomic weight is in atomic mass units.

The Doppler velocity width is related to the half width at half maximum by (Novotny, 1973, eqns 5-18; p 205)

$$\Delta u_{1/2} = (\ln 2)^{1/2} u_{Dop} = 0.832555\, u_{Dop} \quad [\mathrm{cm\ s^{-1}}] \tag{5.15}$$

and the FWHM is given by

$$\Delta u_{FWHM} = 2(\ln 2)^{1/2} u_{Dop} \quad [\mathrm{cm\ s^{-1}}]. \tag{5.16}$$

5.4.4 The Doppler *b* parameter

Much of the literature refers to the Doppler b parameter. This is the Doppler velocity width or velocity dispersion with turbulence included, and is given by

$$b^2 = u_{Dop}^2 = 2kT/m_A + u_{turb}^2 \quad [\mathrm{cm^2 s^{-2}}]. \tag{5.17}$$

With these definitions

$$b = u_{Dop} = \Delta u_{FWHM} / \left[2(\ln 2)^{1/2}\right] \quad [\mathrm{cm\ s^{-1}}]. \tag{5.18}$$

[1] Note that the **turbulence** command accepts u_{turb} in $\mathrm{km\,s^{-1}}$ but converts it into $\mathrm{cm\,s^{-1}}$, the units used throughout the code.

5.4.5 Voigt function

By combining equations 5.1 and 5.3 we can define the optical depth a relative displacement x away from line center as:

$$\tau_\nu(x) = \int_{R_{\rm in}}^{R_{\rm out}} \frac{\pi^{1/2} q_e^2 \lambda\, f_{l,u}}{m_e c u_{\rm Dop}}\, \varphi_\nu(x)\, (n_l - n_u g_l/g_u)\; f(r)\, dr. \tag{5.19}$$

Using this equation, the line center optical depth τ_0 can be defined as $\tau_0 \equiv \tau_\nu(0)$. The relative displacement x is given by equation 5.4 above. In our formalism, the Voigt function is normalized such that the integral is $\sqrt{\pi}$. A schematic approximation for the Voigt function is given by equation 9-61 of Mihalas (1978)

$$\varphi_\nu(x) \approx \exp(-x^2) + a/(\pi^{1/2} x^2). \tag{5.20}$$

Here a is the damping constant. This expression cannot be used in real calculations as it goes to infinity for $x = 0$, but it does convey the general behavior of the Voigt function where for small x it looks like a Gaussian function while for large x it resembles a Lorentzian profile. In CLOUDY we use an enhanced version of the *humlik* algorithm (Wells, 1999) to calculate the Voigt function to a relative precision of at least 2.5×10^{-3} for all values of a and x. For most values of a, the relative accuracy will be better than 10^{-4} though. The value at line center is given by:

$$\varphi_\nu(0) = 1 - \frac{2a}{\sqrt{\pi}} + a^2 + O(a^3)\ (a \to 0). \tag{5.21}$$

The line center optical depth thus depends on a, or more generally on the shape of the line profile, while the mean optical depth does not.

5.4.6 Mean vs. line center optical depths

CLOUDY internally works with line center optical depths throughout (see, for example, Mihalas, 1978). However, mean optical depths are reported in the final printout. Since CLOUDY treats line overlap and also integrates the line optical depth through a medium where the Doppler width will generally be varying, it is not straightforward to convert the line center optical depths used internally to a mean optical depth. To avoid these difficulties, we report a mean optical depth that is exactly a factor $\sqrt{\pi}$ times *larger* than the line center optical depth. This assumes that the Voigt function at line center is $\varphi_\nu(0) \approx 1$. This approximation is OK when the damping parameter a is small, $a \ll 1$ (see equation 5.21), which is generally the case in the IR, optical, and UV wavelength range. However, this approximation breaks down in the X-ray regime where a can be much larger.

5.5 The Einstein coefficients

The dimensionless oscillator strength gf is related to the transition probability A_{ul} [s^{-1}] by

$$g_l f_{l,u} = g_u f_{u,l} = \frac{m_e c \lambda_{cm}^2}{8\pi^2 q_e^2} g_u A_{u,l} = 1.4992 g_u A_{u,l} \lambda_{cm}^2 = 1.4992 \times 10^{-8} g_u A_{u,l} \lambda_{\mu\rm m}^2 \tag{5.22}$$

where $\lambda_{\mu m}$ is the wavelength in micron and λ_{cm} the wavelength in centimeter. The absorption oscillator strength is related to the transition probability by

$$f_{l,u} = \frac{m_e c \lambda_{cm}^2}{8\pi^2 q_e^2} \frac{g_u}{g_l} A_{u,l} = 1.4992 \times 10^{-8} A_{u,l} \lambda_{\mu m}^2 \frac{g_u}{g_l} \tag{5.23}$$

or

$$A_{u,l} = \frac{8\pi^2 q_e^2}{m c \lambda_{cm}^2} \frac{g_l}{g_u} f_{abs} = \frac{f_{l,u}}{1.4992 \times 10^{-8}} \lambda_{\mu m}^{-2} \frac{g_l}{g_u} \quad [\mathrm{s}^{-1}]. \tag{5.24}$$

Combining equations 5.3 and 5.23 we obtain an expression relating the transition probability and the absorption cross section;

$$\begin{aligned} \alpha_\nu &= \frac{\lambda^3 g_u}{8\pi g_l} \frac{A_{u,l}}{\pi^{1/2} u_{Dop}} \varphi_\nu(x) \\ &= \frac{\lambda^3 g_u}{8\pi g_l} \frac{A_{u,l}}{\pi^{1/2} u_{Dop}} \varphi_\nu(x) \qquad [\mathrm{cm}^2]. \\ &= 2.24484 \times 10^{-14} A_{u,l} \lambda_{\mu m}^3 \frac{g_u}{g_l} \frac{\varphi_\nu(x)}{u_{Dop}} \end{aligned} \tag{5.25}$$

The coefficient for induced emission, B_{ul}, is related to A_{ul} by the phase space factor $2h\nu^3/c^2$;

$$A_{u,l} = \frac{2h\nu^3}{c^2} B_{ul} \quad [\mathrm{s}^{-1}] \tag{5.26}$$

and the induced emission and absorption probabilities are related by

$$g_l B_{l,u} = g_u B_{u,l} \tag{5.27}$$

The absorption cross section α_ν is related to $B_{l,u}$ by

$$\alpha_\nu = \frac{hc}{4\pi^{3/2}} \frac{B_{l,u}}{u_{Dop}} \varphi_\nu(x) \quad [\mathrm{cm}^2]. \tag{5.28}$$

In these terms the optical depth increment (equation 5.1) is given by

$$\begin{aligned} d\tau_{l,u} &= \alpha_\nu (n_l - n_u g_l/g_u) f(r)\, dr \\ &= \frac{hc}{4\pi^{3/2}} \frac{B_{l,u}}{u_{Dop}} \varphi_\nu(x) (n_l - n_u g_l/g_u) f(r)\, dr \end{aligned} . \tag{5.29}$$

5.6 Continuum pumping

5.6.1 Photon occupation number

The intensity of a radiation field can be thought of as two parts, the available volume of phase space $2h\nu^3/c^2$ and a dimensionless occupation number η giving the fraction of that space that is filled. Occupation numbers can be larger than unity for photons, which are Bose-Einstein particles.

For reference, the Planck function is given by

$$B_\nu = I_\nu = \frac{F_\nu}{\pi} = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1} \quad [\mathrm{erg\ cm^{-2}\ s^{-1}\ sr^{-1}\ Hz^{-1}}] \tag{5.30}$$

where F_ν is the single-hemisphere emittance from an opaque surface. The photon occupation number of a blackbody is then

$$\eta_\nu = \frac{1}{\exp(h\nu/kT) - 1} \tag{5.31}$$

The dimensionless occupation number for any continuum with a mean intensity J_ν (erg cm^{-2} s^{-1} Hz^{-1} sr^{-1}) at a frequency ν is defined as

$$\eta_\nu \equiv J_\nu / \left(2h\nu^3/c^2\right) \equiv \left[\exp(h\nu/kT_{ex}) - 1\right]^{-1}. \tag{5.32}$$

Here T_{ex} is the excitation temperature of the continuum at the frequency.

5.6.2 Pumping rates

Continuum fluorescence is treated as in Ferland and Rees (1988) and Ferland (1992). The rate of induced radiative excitation by continuum photons (continuum pumping) is given by

$$r_{l,u} = n_l B_{l,u} J_{l,u} = n_l A_{u,l} \frac{J_{l,u}}{2h\nu^3/c^2} \frac{g_u}{g_l} = n_l A_{u,l} \eta_\nu \frac{g_u}{g_l} \quad [\text{cm}^{-3}\ \text{s}^{-1}] \tag{5.33}$$

where η_ν is the dimensionless continuum occupation number at the line energy. The rate of induced radiative de-excitation is related by detailed balance and is given by

$$r_{u,l} = r_{l,u} \frac{g_l}{g_u} \quad [\text{cm}^{-3}\ \text{s}^{-1}]. \tag{5.34}$$

The occupation number has the advantage that the Einstein B's do not enter any rate equations. All radiative rates can be expressed in terms of an A and ν.

5.6.3 Optical depth effects

The line becomes self-shielding when the optical depth is greater than unity. The line optical depth between the current position and the illuminated face of the slab is used to evaluate the inward-looking escape probability, the probability that a line photon will travel this distance in a single scattering. Line optical depths do not directly affect η_c, only continuous opacities do. The final form of the continuum pumping rate is

$$r_{l,u} = n_l A_{u,l} \eta_\nu \frac{g_u}{g_l} \gamma_{l,u}(\tau) \quad [\text{cm}^{-3}\ \text{s}^{-1}] \tag{5.35}$$

where $\gamma_{l,u}$ is the probability that continuum photons penetrate an optical depth τ_o and are then absorbed by an atom:

$$\gamma_{l,u} = \int_0^\infty \varphi_\nu \exp(-\tau_o \varphi_\nu)\, d\nu \Big/ \int_0^\infty \varphi_\nu\, d\nu. \tag{5.36}$$

where φ_ν is the Voigt function. Figure 5.1, taken from Ferland (1992), shows $\gamma_{l,u}$ for a wide variety of values of the damping constant a.

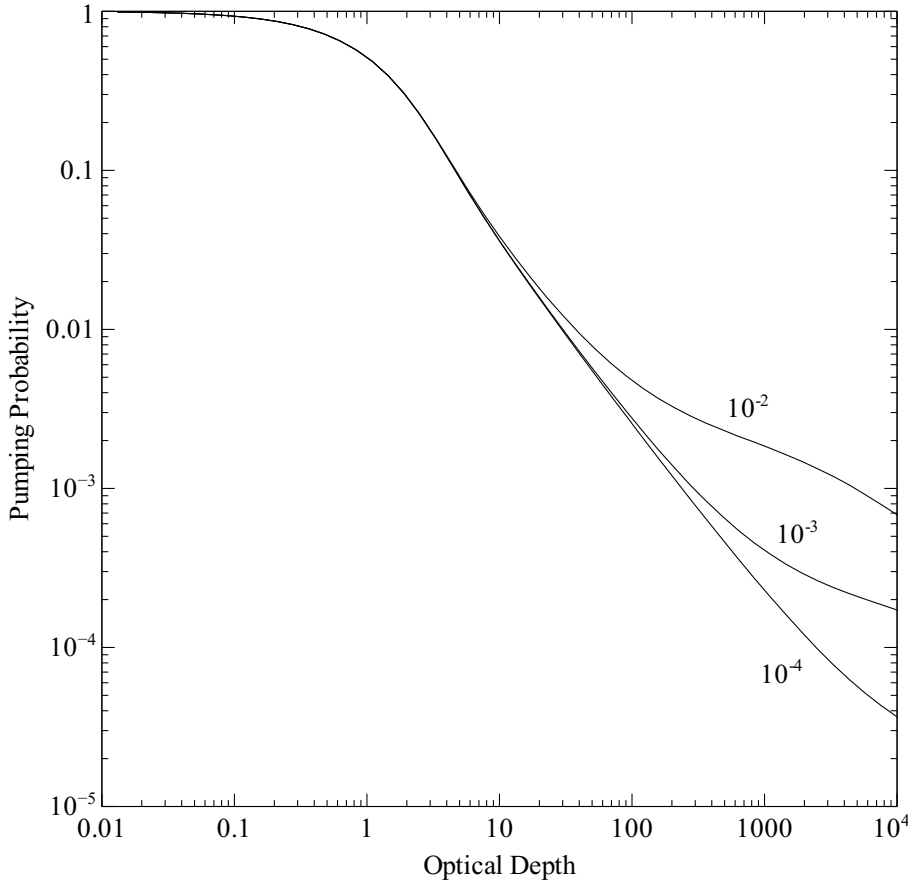

Figure 5.1: This figure shows the probability that a photon will penetrate to the line center optical depth shown on the x-axis, and then be absorbed by the line. The curves are for various values of the damping constant a (the ratio of damping width to Doppler width), as indicated on the figure.

The code works in terms of the flux of photons per energy mesh point. The transmitted continuum has a flux of photons φ_ν (photons cm^{-2} s^{-1} Ryd^{-1}). The photon occupation number of the attenuated continuum is given by equation 5.31 above, here written as

$$\eta_\nu = \varphi_\nu \frac{c^2}{8\pi\, \nu_1^3\, \nu_{Ryd}^2} \tag{5.37}$$

where ν_{Ryd} is the frequency in Rydbergs, ν_1 is the frequency of 1 Rydberg, and the other symbols have their usual meaning. Continuum pumping is included among the general line excitation processes for all lines considered by the code.

5.7 Kirchhoff's Law

Kirchhoff's law is the statement that, in thermodynamic equilibrium, the energy emitted is equal to the energy absorbed. If the emission and absorption coefficients are j_ν and κ_ν then

$$j_\nu = \kappa_\nu B_\nu(T) \tag{5.38}$$

where $B_\nu(T)$ is Planck's function.

5.8 The line source function and mean intensity

The source function for a line is defined as

$$S_l\,(T_{exc}) \equiv B_l\,(T_{exc}) \equiv \frac{j_l}{\kappa_l} = \frac{A_{u,l} n_u}{B_{l,u}\,(n_l - n_u g_l/g_u)} \quad [\text{erg Hz}^{-1}\ \text{sr}^{-1}\ \text{s}^{-1}]. \tag{5.39}$$

where T_{exc} is the line excitation temperature

$$\frac{n_u/g_u}{n_l/g_l} = \exp\left[-h\nu/kT_{exc}\right] \tag{5.40}$$

$B_l(T_{exc})$ is the Planck function at the line excitation temperature and the line emission and absorption coefficients jl and kl enter through Kirchhoff's law. Combining with the definitions of the Einstein relations we find the relation

$$S_l\,(T_{exc}) = \frac{2h\nu^3}{c^2} \frac{n_u/g_u}{(n_l/g_l - n_u/g_u)} \quad [\text{erg Hz}^{-1}\ \text{sr}^{-1}\ \text{s}^{-1}]. \tag{5.41}$$

The radiation field within the line is given by the mean intensity $\bar{J}$. $\bar{J}$ and S_l are related by the net radiative bracket, which we approximate as the escape probability P_{esc}:

$$P_{esc} \equiv 1 - \bar{J}/S_l. \tag{5.42}$$

The mean intensity is then give by

$$\bar{J} = S_l\,(1 - P_{esc})\,. \tag{5.43}$$

and the line center photon occupation number is

$$\eta_l = \frac{n_u/g_u}{(n_l/g_l - n_u/g_u)}\,(1 - P_{esc})\,. \tag{5.44}$$

5.9 Level populations in radiative equilibrium limit

For a two-level system where collisions can be neglected, in the optically thin limit, the balance equation relating the populations of a two-level system is given by

$$\frac{dn_u}{dt} = n_l B_{lu} J - n_u \left(A_{ul} + B_{ul} J\right) \quad [\mathrm{cm}^{-3}\ \mathrm{s}^{-1}]. \tag{5.45}$$

In the time-steady limit, where the time derivative is zero, the balance can be rewritten in terms of the transition probabilities as

$$n_u \left(A_{ul} + A_{ul}\eta\right) = n_u A_{ul} \left(1 + \eta\right) = n_l A_{ul} \eta \frac{g_u}{g_l} \quad [\mathrm{cm}^{-3}\ \mathrm{s}^{-1}]. \tag{5.46}$$

In the limit where η is small every photoexcitation is followed by spontaneous decay, while in the limit where η is large the level populations are given by the ratio of statistical weights, i.e., T_{exc} is infinite.

Chapter 6

LINE DETAILS

6.1 Overview

The effects of optical depths, continuum pumping, collisions, and destruction by background opacity, are computed for *all* permitted and intercombination lines. The cooling is usually distributed among many lines in high-density models, and these lines are usually optically thick. This section describes the methods and data structures used within the code to accomplish this.

6.2 Line Boltzmann factors

The Boltzmann factor $h\nu/kT$ for a line with a known wavelength or energy is given by Table 6.1. The table lists the ratio $h\nu/k$ for various units of the line energy. Vacuum, not air, wavelengths, must be used for all quantities involving wavelengths.

6.3 Air vs vacuum wavelengths

In the past the convention across physics and astronomy was to give line wavelengths in vacuum for $\lambda_{\rm vac} \leq 2000$ Å and in air for $\lambda_{\rm vac} > 2000$ Å. Nowadays it is becoming more usual for (mainly space-based) observatories to produce spectra that use vacuum over the entire wavelength range.

Air wavelengths are smaller than vacuum wavelengths because the wavefronts are crushed as they enter the denser medium with its higher index of refraction. The frequency is unchanged.

Table 6.1: Line Boltzmann Factors

Line Energy Units	$h\nu/k$ (K)
Angstroms	1.43877(+8)/λ(Å)
microns	1.43877(+4)/$\lambda(\mu)$
wavenumbers	1.43877$\times\sigma$
Rydbergs	1.5788866(+5) $\times$E

6.4 The line escape probability functions

6.4.1 Escape probability formalism vs exact radiative transfer

Radiative transport effects are approximated with the escape probability formalism (EPF). This includes line pumping by the incident continuum, photon destruction by collisional deactivation or by continuous opacities, and line overlap in special cases. This section describes how the escape probability is related to the net radiative bracket, the formally correct term in the transfer equation.

The full balance equation for radiative losses and gains for the upper level of a two level atom is given by

$$n_u A_{ul} + n_u B_{ul} \bar{J} - n_l B_{lu} \bar{J} \equiv n_u A_{ul} \rho_{ul} \approx n_u A_{ul} P_{ul} \tag{6.1}$$

where A and B are the Einstein coefficients, $\bar{J}$ is the mean intensity averaged over the line, and $\rho_{\rm ul}$ is the net radiative bracket, defined as

$$\rho_{ul} \equiv 1 - \bar{J}/S \tag{6.2}$$

where S is the line source function. The essence of the EPF is to replace $\rho_{\rm ul}$ with the escape probability P_{ul} on the argument that the difference between J and S is due to photons leaking away from the region. (Elitzur et al., 1983; Sec 2.6) shows that this is exact if S is constant across the line-forming region. In the code $\rho_{\rm ul}$ is replaced with P_{ul}.

6.4.2 Redistribution functions

At low densities, line scattering for a two-level atom is coherent in the atom's reference frame and the line profile function is described by the incomplete redistribution function. At high densities the Stark effect can broaden the line. When the radiation density is high, scattering within excited states can inhibit the broadening of resonance lines such as Lβ (line interlocking), destroying the coherence of the scattering process. In these cases complete redistribution in a Doppler core more closely describes the scattering process.

CLOUDY uses several escape probability functions to take these processes into account. Strong resonance lines are treated with partial redistribution with a Voigt profile. Subordinate lines are treated with complete redistribution in a Doppler core.

6.4.3 Incomplete redistribution

Incomplete redistribution is assumed for resonance transitions such as C IV λ1549 and the Lα transitions of hydrogen and helium. Two studies of line formation using this approximation are those of Bonilha et al. (1979) and Hummer and Kunasz (1980). Both studies suggest escape probabilities of the form

$$P_l(\tau) = \{1 + b(\tau)\ \tau\}^{-1} \tag{6.3}$$

but there is substantial disagreement in the form and value of the factor $b(\tau)$, sometimes by more than a factor of 2. (This is after due allowance for the different definitions of line opacities in the two papers.) CLOUDY uses the Hummer and Kunasz (1980) results for H I, He I, and He II Lα and strong resonance lines such as C IV λ1549. Their tabulated values were fitted by interpolation.

6.4.4 Damping constant

The damping constant a is given by

$$a = \frac{\Gamma}{4\pi\,\Delta\nu_D} = \frac{\lambda_{cm}\sum A}{4\pi\,u_{Dop}} = \frac{\lambda_{cm}7.958\times10^{-2}\sum A}{u_{Dop}} = \frac{\lambda_{\mu m}7.958\times10^{-6}\sum A}{u_{Dop}} \tag{6.4}$$

where Γ is the inverse lifetime of the level (the sum of the A's from the upper level), $\Delta\nu_D$ is the Doppler width in frequency units (Mihalas, 1978), λ_{cm} and $\lambda_{\mu m}$ are the wavelengths in cm and μm respectively, and u_{Dop} is the Doppler width in cm s^{-1}. The ratio $\Gamma\lambda/4\pi$ is stored in the line structures and the a's are evaluated using this ratio and the current Doppler width.

6.4.5 Background opacity and Destruction probability

The ratio of continuous to total opacity is X_c parameterized as

$$X_c = \frac{\sum \kappa_c\, n_c}{\kappa_l n_l + \sum \kappa_c\, n_c} \tag{6.5}$$

where the κ_l's are the line center absorption opacities and the n's the number of absorbers.

6.4.6 Complete redistribution

Lines arising from excited states (hydrogen Balmer, Paschen, etc.) and Lyman lines with $n_u > 2$ are treated assuming complete redistribution in a Doppler core (i.e., the damping constant a is assumed to be zero). This assumption can be changed with the **atom redistribution** command. If the total optical depth of the slab is T, then the escape probability at a depth τ from the illuminated face is given by;

$$P_{u,l}(\tau, T, X_c) = [1 - X_c F(X_c)]\,\frac{1}{2}\,[K_2(\tau, X_c) + K_2(T-\tau, X_c)] \quad , \tag{6.6}$$

and the destruction probability is

$$D_{u,l}(X_c) = X_c F(X_c). \tag{6.7}$$

The function is

$$F(X_c) = \int_{-\infty}^{\infty} \frac{\varphi(x)}{X_c + \varphi(x)}\,dx, \tag{6.8}$$

where in these expressions (and in this part of the code) the *mean opacity is used*, and $\varphi(x) \approx \pi^{1/2}\exp(-x^2)$ is the Voigt function. $F(X_c)$ is interpolated from the tables presented by Hummer (1968). The function

$$K_2(\tau, X_c) \equiv \frac{1}{1 - X_c F(X_c)} \int_{-\infty}^{\infty} \frac{\varphi^2(x)}{X_c + \varphi(x)} E_2\left[(X_c + \varphi(x))\,\tau\right]\,d\tau \tag{6.9}$$

is evaluated numerically.

The complete redistribution escape probabilities are corrected for finite damping parameters by including a separate wing escape probability. The resulting total escape probabilities have been

tested against numerical integrations of the exact formulae in Avrett and Loeser (1966); Hummer and Rybicki (1982) – note the different definitions of K_2 in these papers – verified by comparison by the tabulations and fits in these papers. The overall fit to the escape probability is in error by at most 25% in the range $a = 10^{-3}$–10^{3}, with the largest error at $\tau \simeq 1$, and correct asymptotic behaviour in the low τ and high τ limits. This level of accuracy is thought to be sufficient, given the other approximations inherent in the escape probability method.

6.4.7 Masing lines

A line mases when its optical depth is negative. The escape probability is (Elitzur, 1992; p 32, see also Elitzur, 1990a,b)

$$P_{u,l} = \frac{1-\exp(-\tau)}{\tau}. \tag{6.10}$$

The code will generate a comment if strong maser action occurs for any transition.

6.4.8 Stark broadening

Distant collisions with charged particles broaden the upper levels of lines, and in the limit of very high densities this will make the scattering process completely non-coherent even for Lα (i.e., complete redistribution obtains). Cloudy closely follows the treatment of Puetter (1981) in treating Stark broadening.

6.4.9 Net escape probability

A total escape probability $P_{l,tot}$, given by

$$P_{u,l} = \min\left(P_{inc} + P_{Stark}\ ,\ P_{com}\right), \tag{6.11}$$

is defined for transitions described by incomplete redistribution. The escape probabilities are those for incomplete, Stark, and complete redistribution respectively. The total effective escape probability is not allowed to exceed the complete redistribution value for $\tau > a^{-1}$.

If τ is the optical depth in the direction towards the source of ionizing radiation and T is the total optical depth computed in a previous iteration, then the escape probability entering the balance equations is

$$P_{u,l}(\tau, T) = \left\{P_{u,l}(\tau) + P_{u,l}(T-\tau)\right\}/2. \tag{6.12}$$

In general the total optical depth T is only known after the first iteration, so more than one iteration must be performed when radiative transfer is important.

6.5 Optical depths and the geometry

The terms open and closed geometry are defined in a section in Part I. The treatment of transfer in these two limits is described here.

6.5.1 Open geometry

This is the default. During the first iteration the line optical depth is defined using only optical depths accumulated in the inward direction. This optical depth is initialized to a very small number at the start of the calculation. At the end of the first iteration the total optical depth is set to the optical depth accumulated in the inward direction. At the end of subsequent iterations the total optical depth is defined as a mean of the new and old inward optical depths.

6.5.2 Closed geometry overview

Continuum photons are assumed to interact with gas fully covering the continuum source. At the end of the first iteration the total continuum optical depths are set equal to twice the computed optical depths, and the inner optical depths reset to the computed optical depths. The same recipe is followed on subsequent iterations, except that means of old and newly computed optical depths are used.

Closed expanding geometry This is the default if the **sphere** command is entered. In this case it is assumed that line photons do not interact with lines on the "other" side of the expanding spherical nebula. The treatment of line optical depths is entirely analogous to that described for an open geometry, since the presence of the distant material has no effect on line transfer.

Closed static geometry This is assumed if the **sphere static** command is entered. In this case line photons from all parts of the spherical shell do interact. As a result the optical depth scale is poorly defined on the first iteration, and more than one iteration is required. On second and later iterations the total line optical depth is set to twice the optical depth of the computed structure, and the optical depth at the illuminated face of the shell is set to half of this. The optical depth scale is only reliably defined after at least a second iteration.

6.5.3 Wind

The model is a large velocity gradient ($v \propto R$ Sobolev approximation) wind. This is described further in Part 2 of this document.

6.6 Collision strengths

I have tried to follow the Opacity Project notation throughout this document (Lanzafame et al., 1993). The energy-specific collision strength Ω_{lu} for a transition between upper and lower levels u and l is related to the excitation cross section Q_{lu} by

$$Q_{lu} = \frac{\pi \Omega_{lu}}{g_l k_{lu}^2} \quad [\mathrm{cm}^2] \tag{6.13}$$

where k_{lu}^2 is the wavenumber of the collision energy. If the collisions are with thermal electrons having a Maxwellian velocity distribution $f(u)$ and velocity u then the rate coefficient q_{lu} is given by

$$q_{lu} = \int_0^\infty f(u) u Q_{lu}\, du = \frac{2\pi^{1/2}\hbar^2}{g_l m_e} a_o \left(\frac{R_\infty}{kT}\right) \Upsilon_{lu} \exp\left(-\frac{E_{lu}}{kT}\right) \sqrt{\frac{2kT}{m_e}} \quad [\mathrm{cm}^3\mathrm{s}^{-1}]. \tag{6.14}$$

E_{ul} is the transition energy in Rydbergs, a_o is the Bohr radius,

$$a_o = \frac{\hbar^2}{m_e q_e^2} = 0.529177249 \times 10^{-8} \text{ cm} \tag{6.15}$$

and R_∞ is the Rydberg energy. Then the thermally-averaged collision strength is given by

$$\Upsilon_{lu} = \int_0^\infty \Omega_{lu} \exp\left(-\frac{\varepsilon}{kT}\right)\, d\left(\frac{\varepsilon}{kT}\right). \tag{6.16}$$

The rate coefficient for collisional de-excitation is then given by

$$q_{ul} = \frac{\Upsilon}{g_u\sqrt{T_e}}\left(\frac{2\pi}{k}\right)^{1/2}\frac{\hbar^2}{m_e^{3/2}} = \frac{\Upsilon 8.6291 \times 10^{-6}}{g_u\sqrt{T_e}} \quad [\text{cm}^3\text{s}^{-1}]. \tag{6.17}$$

The rate coefficient for excitation follows from detailed balance:

$$q_{lu} = q_{ul}\frac{g_u}{g_l}\exp(-\chi) = \frac{\Upsilon 8.6291 \times 10^{-6}}{g_l\sqrt{T_e}}\exp(-\chi) \quad [\text{cm}^3\text{s}^{-1}]. \tag{6.18}$$

6.7 Born approximation

The Born approximation is valid for energies much larger than the excitation energy of the transition. The energy specific collision strength is given by Bethe (1930) as

$$\Omega_{lu} \approx \frac{4 g_l f_{lu}}{E_{lu}} \ln\left(\frac{4\varepsilon}{E_{lu}}\right) \tag{6.19}$$

where $f_{l,u}$ is the absorption oscillator strength of the permitted transition.

6.8 The g-bar approximation

The g-bar or van Regemorter (1962) approximation relates the collision strength to the transition probability A_{ul} and wavelength λ (in μm). Here, the collision strength for the downward transition Υ_{ul} is approximately given by

$$\begin{aligned} \Upsilon_{u,l} &= \frac{2\pi}{\sqrt{3}}\frac{m^2e^2}{h^3}\lambda_{\mu m}^3 10^{-12} g_u A_{u,l}\bar{g} \\ &\approx 2.388 \times 10^{-6}\lambda_{\mu m}^3 g_u A_{u,l}\bar{g} \\ &\approx 159\lambda_{\mu m} g_l f_{abs}\bar{g} \end{aligned} \tag{6.20}$$

where g_u and g_l are the statistical weights of the upper and lower levels and f_{abs} is the absorption oscillator strength. For energies of interest in astrophysical plasmas, where $kT < h\nu$, $\bar{g}$ is approximately given by

$$\bar{g} \approx \begin{cases} 0.2; & \text{positive ions} \\ (\text{kT}/\text{h}\nu)/10; & \&\text{neutrals} \end{cases} \tag{6.21}$$

(van Regemorter 1962). These approximations are generally accurate to better than 1 dex. Gaetz and Salpeter (1983) give improved forms of the approximation.

6.9 The critical density

The critical density is defined as the density at which the radiative de-excitation rate $A_{ul}P_{ul}$ (where A is the transition probability and P is the escape probability) equals the collisional de-excitation rate $q_{ul}n_e$. Setting

$$A_{ul}P_{ul} = C_{ul} = q_{ul}n_e = \Upsilon\frac{8.629\times10^{-6}}{g_u\sqrt{T_e}}n_e \quad [\mathrm{s}^{-1}] \tag{6.22}$$

where Υ is the thermally averaged collision strength, the critical density is given by

$$n_{crit} \sim \frac{A_{ul}P_{ul}g_u\sqrt{T_e}}{\Upsilon 8.629\times10^{-6}} \quad [\mathrm{cm}^{-3}]. \tag{6.23}$$

For an optically allowed transition, in which the g-bar approximation may apply, this density is approximately given by

$$n_{crit} = \frac{4.8\times10^{10}\sqrt{T_e}}{\lambda^3_{\mu m}\bar{g}} \quad [\mathrm{cm}^{-3}]. \tag{6.24}$$

6.10 Line thermalization length

Line radiative transfer will affect the thermal equilibrium of the gas when the collision time scale approaches an effective lifetime $\tau \sim A_{ul}/n_{scat})^{-1}$, where A_{ul} is the transition probability and n_{scat} is the number of scatterings a line photon undergoes before escape. For permitted metal lines (which often have optical depths $\sim 10^4 - 10^6$) line thermalization becomes important at densities $n_e > 10^{15}/\tau 10^{10}\mathrm{cm}^{-3}$. These effects are important for hydrogen at considerably lower densities due to its greater abundance. Additionally, continuum transfer affects the ionization and thermal equilibrium of the gas at all densities.

6.11 Averaging levels into terms

6.11.1 Collision strengths

Often cases are encountered in which a multiplet consisting of many lines can be treated as the equivalent two-level atom with a single transition. In these cases it is necessary to define "effective" collision strengths and transition probabilities. If the collision strength from an individual level i is Υ_i, and the statistical weights of the level and term are g_i and g_{tot} respectively, then the effective collision strength Υ_{eff} is related to Υ_i by a simple argument. The collision rate q_i is proportional to the ratio

$$n_i q_i \propto n_i\frac{\Upsilon_i}{g_i} \quad [\mathrm{s}^{-1}] \tag{6.25}$$

so that

$$n_{tot}\, q_{tot} = \sum_i n_i q_i \propto \sum_i n_i\frac{\Upsilon_i}{g_i} \quad [\mathrm{s}^{-1}]. \tag{6.26}$$

In many cases it is valid to assume that the levels within the term are populated according to their statistical weight, viz.,

$$n_i = n_{tot}\frac{g_i}{g_{tot}} \quad [\mathrm{cm}^{-3}]. \tag{6.27}$$

Then, the effective collision strength Υ_{tot} is operationally defined by the relations

$$n_{tot}\frac{\Upsilon_{tot}}{g_{tot}} = \sum_i n_i\frac{\Upsilon_i}{g_i} = n_{tot}\sum_i \frac{g_i}{g_{tot}}\frac{\Upsilon_i}{g_i} = n_{tot}\frac{\sum_i \Upsilon_i}{g_{tot}}. \tag{6.28}$$

So, the effective collision strength of the entire multiplet is

$$\Upsilon_{tot} = \sum_i \Upsilon_i. \tag{6.29}$$

6.11.2 Transition probabilities

Under similar circumstances an effective transition probability A_{eff} may be defined as

$$n_{tot}A_{tot} = \sum_i n_i A_i = n_{tot}\sum_i \frac{g_i}{g_{tot}}A_i \tag{6.30}$$

so that the effective transition probability is

$$A_{tot} = \sum_i \frac{g_i}{g_{tot}}A_i. \tag{6.31}$$

So collision strengths are added, and transition probabilities averaged.

6.12 Level populations with collisions

Both escape and destruction probabilities enter in the calculation of a level population and line emissivity. The escape probability $P_{u,l}$ is the probability that a line photon will escape in a single scattering (Elitzur et al., 1983; Elitzur, 1984). The destruction probability $D_{u,l}$ is the probability that a line photon will be destroyed in a single scattering.

The line de-excitation rate is given by

$$\left(\frac{dn_u}{dt}\right)_{rad} = n_u A_{u,l}\left(P_{u,l}+D_{u,l}\right) - n_l A_{u,l}\eta\gamma_{u,l} + n_u C_{ul} - n_l C_{lu} \quad [\mathrm{cm}^{-3}\mathrm{s}^{-1}] \tag{6.32}$$

where η is the photon occupation number of the attenuated external radiation field, C is the collision rate (s^{-1}), and $\gamma_{u,l}$ is the fluorescence probability.

The net emission from a transition between the level n to a lower level l and escaping to the surface is then

$$4\pi\, j(n,l) = n_n A_{n,l}\, h\nu_{n,l}\, P_{u,l}(\tau_{n,l})\, f(r) \quad [\mathrm{erg\ cm}^{-3}\mathrm{s}^{-1}] \tag{6.33}$$

where $f(r)$ is the filling factor. The total emission from the gas is then

$$e(n,l) = \int_V n_n A_{n,l}\, h\nu_{n,l}\, P_{u,l}(\tau_{n,l})\, f(r)\, dV \quad [\mathrm{erg\ cm}^{-2}\mathrm{s}^{-1}\,\mathrm{or\,erg\,s}^{-1}] \tag{6.34}$$

depending on whether the intensity or luminosity case is chosen. The local cooling rate (erg cm^{-3} s^{-1}) due to the line is related to the level populations by

$$\Lambda_{u,l} = \left(n_l C_{l,u} - n_u C_{u,l}\right)\ f(r)\ h\nu \quad [\mathrm{erg\ cm^{-3} s^{-1}}] \tag{6.35}$$

and the local flux (cm^{-2} s^{-1}) of "on-the-spot" (OTS) photons caused by line loss (used to compute heating or photoionization rates for the sources of the background opacity) is

$$\varphi_{OTS} = \frac{n_u A_{u,l} D_{u,l}(X_c)}{\sum \kappa_c\, n(c)}. \tag{6.36}$$

The ratio of inward to total line intensity is then given by

$$\frac{4\pi\, j(in)}{4\pi\, j(total)} = \frac{P_{u,l}\,(\tau)}{\left[P_{u,l}\,(\tau) + P_{u,l}\,(T-\tau)\right]}. \tag{6.37}$$

Chapter 7

CLOUDY AS A STANDALONE PROGRAM

CLOUDY can be used to run a single model, to create large grids of calculations, or to compute a number of simulations while varying one or more parameters to match an observed spectrum. This Chapter describes how to use CLOUDY as a self-contained program to read in the parameters for the simulation and compute the result. The next Chapter discusses the case in which the code is called as a subroutine of another larger code.

7.1 Running a single model with a shell script

The code reads from an input file and can create a large number of output files. The latter include both the main output (described in Chapter 1, *OUTPUT*) and the ancillary "save" files (described in the Chapter 16 of Hazy 1, *CONTROLLING OUTPUT*).

It is a good idea to follow a naming convention for these files. The convention I use is the style "`basename.type`" where `basename` explains the astrophysical context (for instance, "quasar" or "IGM") and `type` gives the type of information in the file. For instance, a model of a planetary nebula may have the base name "`pn_halo`", the input script might be `pn_halo.in`, the output would be in `pn_halo.out`, and the file created by the **save overview** command might be `pn_halo.ovr`. Then all of these files could be located with a simple "**ls pn**.*" and all overview files with a "**ls *.ovr**" on a Linux system.

The `pn.in` file contains the input commands that tell the program what to do. A typical example might be the following:

```
# log of the hydrogen density (cm^-3)
hden 4
# log of the inner radius (cm)
radius 17
# black body temperature and total luminosity
black body 1e5 K, luminosity 38
save overview "pn.ovr"
```

CLOUDY stops reading the input steam when it reaches either an empty line or the end of file. Nothing special is needed at the end of the input file.

I have a shell script named `run` which is in my "`bin`" directory, which I include on my path. The shell script `run` consists of the following on Linux:

```
cloudy.exe < $1.in > $1.out
```

Under Windows it would have the name `run.bat` and would contain the following

```
cloudy.exe < %1.in > %1.out
```

If `run` is executed by typing

```
run pn
```

it would read the input stream in `pn.in` and create an output file called `pn.out`.

7.2 Running a single model from the command line

The code also has two command-line options that will accomplish the same thing as the shell script described in the previous section. If you create an executable called `cloudy.exe`, then the command

```
cloudy.exe model.in
```

will read input from `model.in`, write output to `model.out`, and add the prefix `model` to all the save files. This can also be written

```
cloudy.exe -p model
```

Alternatively, you can use the command

```
cloudy.exe -r model
```

which does the same thing, except that it will *not* add the prefix `model` to all the save files (mnemonic: `-p` will Prefix Save file names, while `-r` will only Redirect input and output).

By typing the command

```
cloudy.exe -h
```

you can a list of all the command line flags that CLOUDY supports. There are two additional flags, **-a** and **-g**, that are used for debugging the code and internally in grid runs. They should never be used in normal situations.

7.3 Running grids of simulations or optimizing a simulation

The greatest insight is gained by creating grids of simulations which vary one or more of the input parameters to show how various predictions change, or to optimize the agreement between the predicted and observed values. One example, the predicted C IV *lambda*1549 equivalent width as a function of the flux of ionizing photons and cloud density, is shown in Figure 8.1. See Baldwin et al. (1995c) for more details.

Such grids of simulations can be made parallel on distributed memory parallel machines because each point in the grid is independent of the other points.

7.3.1 Grids of simulations

The **grid** command is described in Chapter 18 *THE GRID COMMAND* of Hazy 1.

7.3.2 Optimizing a simulation

The **optimize** command is described in Chapter 17 *THE OPTIMIZE COMMAND* of Hazy 1.

7.4 Parallel processing with MPI

Peter van Hoof created a wrapper for the **grid** and **optimize** commands. CLOUDY will automatically run these commands using all available processors if the code is compiled with an MPI aware compiler and run on an appropriate computer.

Chapter 8

CLOUDY AS A SUBROUTINE

8.1 Overview

CLOUDY is designed to be used as a subroutine of other, much larger, codes. When used this way a series of subroutine calls, described next, are used to initialize the code, specify the initial conditions, do the simulation, and finally examine the predictions.

A common strategy is to call the code to compute line intensities for a large matrix of parameters. The results of one such calculation is shown in Figure 8.1 (Baldwin et al., 1995b; Ferland, 2003). Such grids can be computed in a few dozen hours on modern workstations, and offer far greater insight to physical effects of changing model parameters than does a single model.

Much of this can be done without writing a program, by using the **grid** command. This command was introduced by Ryan Porter in C07.02, and makes it possible to create large grids of models like those shown in Figure 8.1 with commands. The **grid** command is described in Part 1 of this document. There are several **save** output commands that are designed to save information from grid calculations.

8.1.1 Host languages

CLOUDY is written in C++, and it assumed for most of this section that CLOUDY will be called from an external C or C++ program.

However, there is experimental support for a number of other languages.

You can call a C++ program like CLOUDY from a Fortran program by using the ***cfortran.h*** header file described at `http://www-zeus.desy.de/~burow/cfortran/`. I have never tried this. Good luck.

In the subdirectory `sys_gcc_shared`, an additional set of Makefile targets are set up to use the subroutine API described below for Perl and Python scripts, using the SWIG interface generator. In this directory, there is also an experimental direct interface to the Lua scripting language.

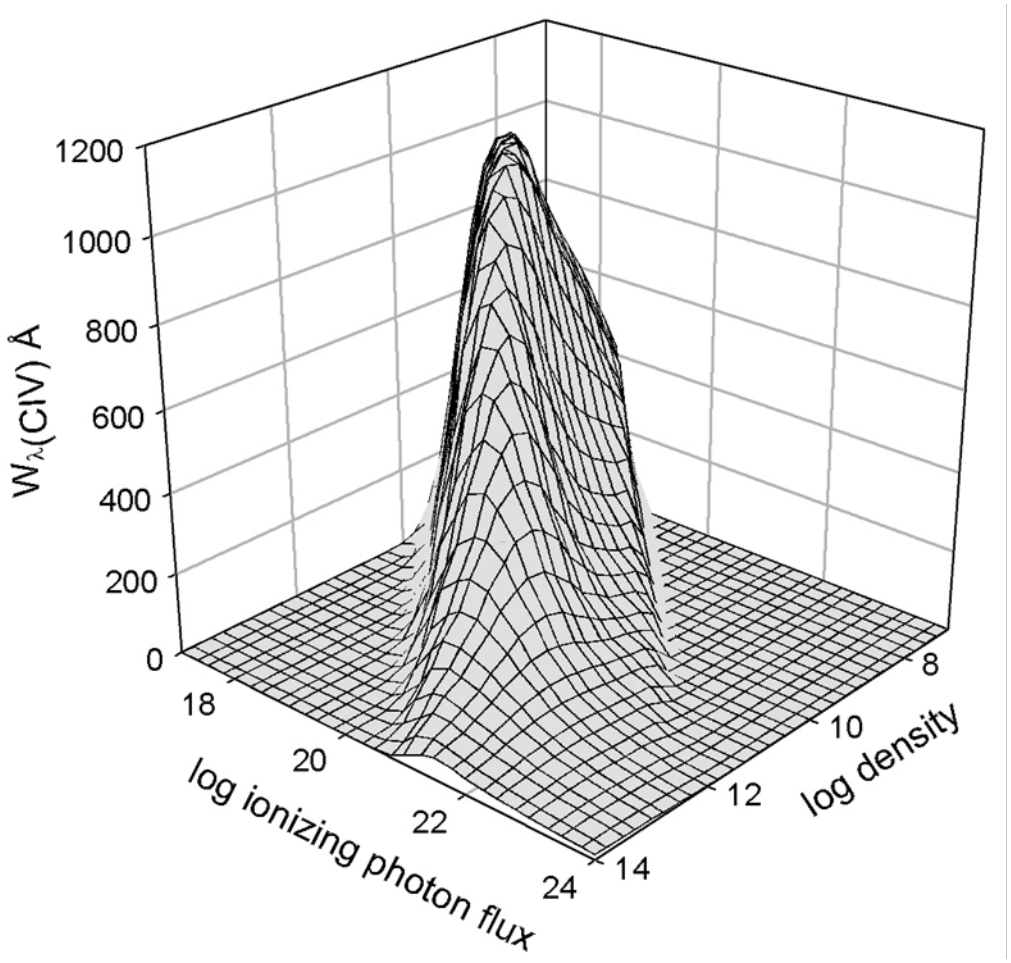

Figure 8.1: The results of a large grid of quasar emission-line cloud calculations are shown. The *x*-*y* plane shows the logs of the hydrogen density ($cm^{3)}$ and flux of ionizing photons (cm^{-2} s^{-1}). The *z* axis is the predicted line equivalent width.

8.1.2 Creating a new main program

In C++ there must be exactly one main program and it must be called *main*. This routine is within the file `maincl.cpp` in the source downloaded from the web. You need to replace the existing CLOUDY main program with one that you write. The file `maincl.cpp` that is included in the distribution must be deleted so that the program you write will be loaded instead. The remaining routines are then compiled with a command like the following:

```
g++ -O3 -c *.cpp
```

which will create a large number of object files. The new main program will then need to be linked with these object files with a command something like

```
g++ -O3 -o mycloudy.exe newmain.cpp *.o -lm
```

Alternatively, if you are using the Makefile build process and have already built CLOUDY, you can use the library file `libcloudy.a` which contains all the object files with the command

```
g++ -O3 -o mycloudy.exe newmain.cpp -L. -lcloudy -lm
```

The following subsections outline how to write code for this new main program.

8.1.3 The cddefines.h and cddrive.h header files

The file `cddrive.h` contains definitions of all public routines, the routines that a user would call to drive CLOUDY. That file is the definitive reference for the material contained in this section and is more up to date than this document. Comments within that file explain all routines and their parameters.

The header `cddefines.h` should come before `cddrive.h` since it includes many definitions and includes the standard C++ header files that are needed to drive the code. The first two header files in the new main routine should be the following:

```
#include "cddefines.h"
#include "cddrive.h"
```

8.1.4 The template for main programs

C++ exceptions are used by CLOUDY. The main program must catch these exceptions. If it does not then the code will crash with an unhandled exception and output files will not be complete. This requires that the main program start with a C++ "try" block and that exception handlers be included within the main program. The adventurous user may enjoy creating their own try block/exception handlers.

A sample template, in the file `template.cpp`, includes the needed code and can be used to create your own programs. It is included in the `programs` directory below the `tsuite` directory in the program download. That version includes a simple call to run the code's smoke test. You would replace the existing code with your own.

8.1.5 A note on return conditions

Some of the routines return a value to indicate success or failure. I try to follow the C and Unix conventions to indicate success with zero (or *false*) and trouble with a non-zero return (or *true*). This rule is not always followed (it is not followed by the important routine *cdLine*), however, and `cddrive.h` should be consulted to make sure the return conditions are understood.

8.2 Initializing the code

Many variables must be initialized at the beginning of the calculation. Calling routine *cdInit* does this.

```
cdInit();
```

Routine *cdInit* must be called every time a new calculation is to be performed, *before* calling any of the following subroutines, but after the results of any previous calculations have been read. (The results of any previous calculations are lost when *cdInit* is called.)

8.3 Handling input and output

8.3.1 cdTalk—produce output?

CLOUDY normally speaks what's on its mind. This would generate too much output in a large grid. It does have a quiet mode in which nothing at all is printed. This quiet mode is set by the logical argument to subroutine *cdTalk*.

```
#include "cddefines.h"
#include "cddrive.h"
cdInit();
/*set no output at all*/
cdTalk( false )
/*have the code produce the normal printout*/
cdTalk( true )
```

The default is for CLOUDY to produce output. *cdTalk* does not have to be called if this is what you want. It needs to be called with the logical variable *false* if the quiet mode is desired.

8.3.2 cdOutput—sending output to a file

CLOUDY normally writes its standard output on the system's `stdout`. This can be changed to another file by calling the routine *cdOutput*, which has two arguments. The first is the name of the file, and the second the mode with which the file should be opened (this is identical to the second parameter of the fopen() routine). Both parameters have default values. The default mode for opening the file is "w", while the default filename is the empty string. Supplying an empty string as the file name means that the output will be directed back to `stdout` again. The output file will be automatically closed on exit of the program. If you call *cdOutput* multiple times with different file names, the file from the previous call will also be closed automatically. The new output file needs to be in the local directory, i.e., writing to a subdirectory or an absolute path is not allowed.

```
#include "cddefines.h"
#include "cddrive.h"

/* open the file output.txt for writing with mode "w" */
/* this will overwrite an existing file */
cdOutput("output.txt");

/* if you want to append to a file, use this instead */
cdOutput("output.txt","a");

/* this will close output.txt and open output2.txt with mode "w" */
cdOutput("output2.txt");

/* if you now want to redirect to stdout again, use this */
/* this will close output2.txt */
cdOutput();
```

8.3.3 cdInput—reading input from a file

CLOUDY normally reads input from the system's `stdin`. This can be changed to another file by calling the routine *cdInput*, which works the same way as the *cdOutput* command described above with the following two exceptions: the default open mode is "r", and supplying an empty string as the file name redirects input back to `stdin`.

8.3.4 cdRead—entering Commands

Command lines are entered by successive calls to the routine *cdRead*. The argument of *cdRead* is a string containing valid commands. These commands must obey all the rules outlined in Part 1.

In the examples below some commands are directly entered as strings (this works when the string is a constant) while other strings are created by writing variables through *sprintf* (a standard C I/O function) or the C++ container ostringstream. C++ I/O has the advantage that you do not have to worry if your buffer is big enough to hold the input line, but otherwise both methods should work equally well. Using either of these methods is necessary when the value of a variable needs to be placed into a string.

```
char chLine[200];/* this string will hold the command lines we will generate*/

/* this example sends the string straight to cdRead */
cdRead( "title a series of constant pressure models" );

/* write variable to a string, then send the string to cdRead */
hden = 5.4;
sprintf( chLine, "hden %5.2f", hden );
cdRead( chLine );

/* this example sends a string that contains double quotes,
 * and so we must "escape" them with backslashes */
cdRead( "save overview \"test.ovr\"" );

/* here we use C++-style I/O as an alternative */
ostringstream oss;
```

```
  oss << "coronal " << temp ;
  cdRead( oss.str() );

  cdRead( "stop zone 1" );
```

You can enter as many input lines as you need. There is no limit other than what the amount of memory on your computer can hold. *cdRead* returns an int that always holds the value *INT_MAX* [1]. The return value was ignored in the examples above.

8.4 Executing the code

8.4.1 cdDrive—calling the Code

The calculation is performed when routine *cdDrive* is called. *cdDrive* returns a bool indicating whether the calculation aborted. The value *false* indicates a successful calculation. The following shows an example of its use.

```
if( cdDrive() )
{
    printf("problems!\n");
    cdEXIT(EXIT_FAILURE);
}
```

If problems occurred and the results cannot be trusted then the return value is *true*. This will only be set if the calculation suffered a complete meltdown. Routine *cdNwcns* can be called to find out about any problems.

8.4.2 cdNoExec—checking without Computing

If routine *cdNoExec* is called after *cdInit* but before *cdDrive* then only the initial parts of a calculation will be performed when routine *cdDrive* is called.

```
cdInit();

/*read in commands */
cdRead( . . .);

/*tell it not to execute */
cdNoExec();

/*call the code */
if( cdDrive() )
    cdEXIT(EXIT_FAILURE);
```

When *cdDrive* is called after *cdNoExec* the code will generate the incident continuum, set the initial density, and derive the chemical composition. It will then stop just before the initial search

[1] In versions C17 and earlier the return value indicated how many lines could still be entered. Now that the restriction on the number of input lines has been lifted, this return value is no longer needed, but has been retained for backward compatibility.

for the physical conditions in the first zone. All of the initial printout, summarizing properties of the composition and continuum, will be generated. This provides a quick way to check that a large grid of models will be specified correctly without actually fully computing the grid.

8.5 Ending the code

The code must end by calling *cdEXIT*. This routine will close any open output files and do other needed jobs before exiting. The full output may not be produced if this routine is not called. Routine *cdEXIT* takes a single parameter, *EXIT_SUCCESS* or *EXIT_FAILURE*, standard macros that indicate how the program ended.

The routine *cdEXIT* is a pair with *DEBUG_ENTRY*. Any routine that calls *cdEXIT* must also have a call to *DEBUG_ENTRY* statement at the start. The routine *DEBUG_ENTRY* has a single parameter, a string giving the name of the routine (which should be "main()") in the case of the main program.

8.6 Checking Predictions

This section describes a series of routines that allow predicted quantities to be obtained after the calculation is complete.

8.6.1 cdB21cm—mean magnetic field

The return value is the mean magnetic field weighted by $n(\mathrm{H}^0)dr/T_{spin}$. This is related to the field measured with 21 cm Zeeman observations. A tangled magnetic field is assumed. A magnetic field is not included by default but can be added with the **magnetic field** command, described in Part 1 of this document.

8.6.2 cdColm—the computed column densities

The predicted column densities of some species can be obtained by calling routine *cdColm*:

```
/* want N(C+2) */
if(cdColm("carb", 3 , &column))
{
    printf(" could not find C+2\n");
}
else
{
    printf("The predicted C+2 column density is %e\n", column );
}
```

The routine returns zero if it found the species, and 1 if it could not. It returns the predicted column density [cm^{-2}] as the third argument. The first argument *chLabel* is a four-character string that must agree with the first four characters (upper or lower case) of the name used to indicate the element in the printout. The second (integer) variable *ion* is the spectroscopic designation of the level of ionization, i.e., 1 indicates the atom C^0, 3 indicates C^{+2}, etc.

Table 8.1: Special cases and examples, cdColm Column Densities

Excited states		molecules
Label	Level	Label
He1*	$He^0\ 2^3S$	H2
C+1[2]	$C^+ J = 3/2$	H-
C[1]	$C^0 J = 0$	H2+
C[2]	$C^0 J = 1$	H3+
C[3]	$C^0 J = 2$	H2g
C+2[2]	$C^{2+} J = 0$	H2*
C+2[3]	$C^{2+} J = 1$	HeH+
C+2[4]	$C^{2+} J = 2$	CO
O[1]	$O^0 J = 2$	OH
O[2]	$O^0 J = 1$	H2O
O[3]	$O^0 J = 0$	O2
Si+[1]	$Si^+ J = 3/2$	SiO
		H-
		C2
		C3
		CN
		CH
		CH^+
H2vJ	H_2 any v, J	H2

The ion stage of 0 indicates a special case, a molecule or an excited level of an atom or ion. The label determines the species in this case. Molecules with names less than 4 characters can be accessed by this route, as well as ions with their chemical designation (e.g. `C+` for C^+). `H2` accesses the total H_2 density, `H2g` and `H2*` access the ground and excited state densities. If the label is shorter than four characters, padding the string with spaces is optional for backward compatibility[2].

If the label has at the end a number contained in square brackets, e.g. `C+[2]`, then the column density is printed for the species excitation level with this index. The index of the level is as given in the corresponding data file. So `C+[2]` is the level with index 2 of the C^+ ion. Certain special cases can also be accessed if the fourth character is a `*`, in particular `Si2*` and `He1*` as documented in Table 8.1.

A large and complex model of the H_2 molecule is computed when the **atom H2** command is included. It is possible to obtain column densities in any v, J level of H_2 by calling routine ***cdH2_colden***.

8.6.3 cdCooling_last—last zone's cooling

The return value is the total cooling rate (erg cm^{-3} s^{-1}) for the last computed zone.

[2]In version C13 and before, the label string had to be exactly 4 characters long at all times.

8.6.4 cdDepth_depth—the depth structure of the cloud

This routine returns a vector giving the zone depths (in cm) of the previous iteration. The code uses adaptive logic to control the radial zoning of the model. Neither the number of depth points nor their structure is known in advance. This routine is called with a double precision vector with enough space to hold the structure. The number of depth points is determined by calling *cdnZone* and space must be allocated by the calling routine. Each element of the vector is the depth from the illuminated face to the center of zone *n*.

8.6.5 cdEDEN_last—electron density of last zone

This returns the electron density (cm^{-3}) of the last zone.

8.6.6 cdEmis—emissivity of lines

cdEmis has the same arguments as *cdLine* but returns the local emissivity (erg cm^{-3} s^{-1} for unit filling factor) of the line for the last computed zone. The return value is the index of the line within the line stack if it was found, and the negative of the number of lines in the stack if the line could not be found.

8.6.7 cdGetLineList—sets of emission lines

The routine *cdGetLineList* provides a way to automatically access a list of emission lines.

First enter a list of emission lines into a file. The format is described in Sect. 16.68.7 of Part 1 of this document. A set of such files is included in the data directory of the distribution files. They have names `LineList*.dat`. You can use these as examples to create your own files.

The first argument to routine *cdGetLineList* is the name of the file containing the line list. If a null string is passed ("") then `LineList_BLR.dat` is used.

cdInit must be called before *cdGetLineList* is called. Next *cdGetLineList* is called, and finally, the actual grid of calculations begins. The predicted intensities of a set of lines are then extracted by calling *cdLine*.

The second parameter is a vector that is defined by the calling program. When the routine *cdGetLineList* is called it uses this vector to store the line identifications. The function returns the number of lines in the list. If problems occurred then -1 is returned.

The following shows an example of getting the lines from `LineList_NLR.dat`, executing the code, and then obtaining the predicted intensities of all lines listed in `LineList_NLR.dat` by calling *cdLine*.

```
#include "cddefines.h"
#include "cddrive.h"
#include "lines.h"
/* define variables */
exit_type exit_status = EXIT_SUCCESS;
vector<LineID> lineids;
/* initialize the code */
cdInit();
/* get list of lines from a line list included in the distribution */
```

```
long nLines;
if( (nLines=cdGetLineList("LineList_NLR.dat",lineids)) < 0 )
{
    /* this is the error exit - could not obtain the lines */
    cdEXIT(EXIT_FAILURE);
}
/* missing commands here, then call the code */
- - - - - - missing code
if( cdDrive() )
    exit_status = EXIT_FAILURE;
- - - - - - missing commands go here
/* now print the predicted emission line intensities */
for( long n=0; n < nLines; ++n )
{
    double relative, absolute;
    if( cdLine( lineids[n], &relative, &absolute ) < 0 )
    {
        fprintf(stderr,"did not find %s\n",lineids[n].str().c_str());
    }
    print("%.3e\n", relative);
}
cdEXIT(exit_status);
```

8.6.8 cdH2_colden—state-specific column densities of H_2

This returns the column density of any level in the X ground electronic state of H_2. This command only works when the large H_2 molecule is included with the **atom H2** command. It has two integer arguments, the vibration and rotation quantum numbers of a level in X. If both are zero or greater the routine returns the column density in that level. If the vibration quantum number is negative then a summed column density is turned. If $v < 0$ and $J = 0$ it returns the total H_2 column density, if $J = 1$ it returns the ortho column density, and if $J = 2$ the para column density. If the indices do not make sense the routine prints a message and returns -1.

Here are some examples:

```
/* total H2 column density */
total = cdH2_colden( -1 , 0 );
/* ortho column density */
ortho = cdH2_colden( -1 , 1 );
/* para column density */
para = cdH2_colden( -1 , 2 );
/* column density in 0, 0 */
total00 = cdH2_colden( 0 , 0 );
```

8.6.9 cdH2_Line—an H_2 emission line intensity

More than half a million H_2 lines are predicted and there will be instances where two H_2 lines have nearly the same wavelength. Identification of a particular transition within the list of lines can be ambiguous. This command finds the intensity and luminosity of a transition by specifying its upper and lower n,v,J levels. The first six arguments give the n,v,J indices of the upper and lower levels in that order. The last two variables are double pointers that return the intensity and

luminosity of the transition. The function returns 1 if it finds the line and 0 if it did not. (This behavior follows that of *cdLine* rather than the standard C++ conventions on function return values.) Currently this only works for the ground electronic state.

Here is an example:

```
double xInten , xLumin;
/* the 1-0 S(1) at 2.121 microns */
if( cdH2_Lines( 0,1,3 , 0,0,1 , &xInten , &xLumin ) == 0 )
{
    printf("could not find line.\n");
}
```

8.6.10 cdHeating_last—last zone's heating

The total heating rate (erg cm^{-3} s^{-1}) for the last computed zone is returned.

8.6.11 cdIonFrac—the computed ionization fractions

The predicted ionization fractions,[3] averaged over radius, area, or volume, can be accessed by calling the subroutine *cdIonFrac*. The average over radius is defined as

$$\left\langle \frac{n(S^{+n})}{n(S_{gas})} \right\rangle = \frac{\int n(S^{+n})\, f(l)\, dl}{\int n(S_{gas})\, f(l)\, dl} \tag{8.1}$$

where $n(S_{gas})$ is the total gas phase density of the element. The average over area is defined as

$$\left\langle \frac{n(S^{+n})}{n(S_{gas})} \right\rangle = \frac{\int n(S^{+n})\, f(r)\, r\, dr}{\int n(S_{gas})\, f(r)\, r\, dr}. \tag{8.2}$$

The average over volume is defined as

$$\left\langle \frac{n(S^{+n})}{n(S_{gas})} \right\rangle = \frac{\int n(S^{+n})\, f(r)\, r^2\, dr}{\int n(S_{gas})\, f(r)\, r^2\, dr}. \tag{8.3}$$

Two sample calls to the routine follow:

```
/* false below means to not include electrons in the mean */
if( cdIonFrac("carb", 2, &frac, "radius", false) )
{
    cdEXIT(EXIT_FAILURE);
}
printf("The predicted ionization fraction over radius is %g\n", frac);
/* true below means to include electrons in the mean */
if( cdIonFrac("carb", 2, &frac, "radius", true) )
{
    cdEXIT(EXIT_FAILURE);
}
printf("Ionization fraction wrt radius end elec den is %g\n", frac);
```

[3] 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 molecules.

The first argument is a four-character identifier that must agree with the first four characters (upper or lower case) used to indicate the element in the printout. The second integer argument is the spectroscopic designation of the level of ionization, i.e., 1 indicates C^0, 3 indicates the second ion C^{+2}, etc. The third argument returns the predicted ionization fraction S^{+n}/S_{gas}. The 4th argument is a six-character variable (plus end of string sentinel) which must be either "*radius*", "*area*", or "*volume*" (either upper or lower case). This string determines whether the ionization fraction returned is weighted with respect to radius, area, or volume. These would be appropriate to compare to pencil beam observations, integrated long slit observations, or observations of the whole nebula, respectively. The last argument determines whether (*true*) or not (*false*) the ionization fraction is also weighted with respect to the electron density. The function returns zero if the ion was found and non-zero if an error occurred.

An ionization stage of zero will request the fraction of an element within a molecule. If the element name is "H2", then the fraction of hydrogen in H_2, $2n(H_2)/n(H_{tot})$, will be returned. Currently only H_2 is implemented. In this case, padding the string "H2" with spaces is optional for backward compatibility[4].

8.6.12 cdLine—emission-line intensities

This finds the intensity or luminosity of any line. The label and wavelength of the line are specified and the routine returns the relative intensity and the absolute intensity or luminosity. The following is an example.

```
#include "cddefines.h"
#include "cddrive.h"
double relint, absint;
long nType = 0;

if( cdLine( "H  1", 4861.32_air, &relint, &absint, nType ) < 0 )
    printf("did not find this line\n");
// alternate forms
realnum wlHbeta = 4861.32_r;
if( cdLine( "H  1", t_air(wlHbeta), &relint, &absint, nType ) < 0 )
    printf("did not find this line\n");
t_wavl twHbeta = 4861.32_air;
if( cdLine( "H  1", twHbeta, &relint, &absint, nType ) < 0 )
    printf("did not find this line\n");
```

The first argument in the call is the line label, the string (upper or lower case) used by the code to identify the line in the main emission-line printout. The second variable gives the wavelength of the line in angstrom. An extension "_air" or "_vac" should be appended to the literal number to indicate whether it is an air or vacuum wavelength. If you are using variables, you can use the syntax "t_air(var)" or "t_vac(var)" instead, or use a variable of type t_wavl. Both the label and wavelength must exactly match the ones used by CLOUDY to identify the line (see the chapter *Lines* for a full description). The third variable (*relint* in the above example) is a double-precision pointer to the relative intensity of the line (relative to the normalization line, usually Hβ, and reset with the **normalize** command). The intensity (erg cm^{-2} s^{-1}) or luminosity (erg s^{-1}) of the line is

[4] In version C13 and before, the label string had to be exactly 4 characters long at all times.

returned as the fourth double-precision pointer (*absint* in the above example). If the intensity of the line is zero or the line was not found then this variable will be set to 0.

The last (optional) parameter indicates which type of line prediction to return. The integer types are 0 intrinsic, 1 emergent, 2 intrinsic cumulative, 3 emergent cumulative intensities.

The intensities returned when the last parameter is missing or it is zero are those printed with the heading *Intrinsic Intensities*. This does not include the effects of possible reflection off a background molecular cloud or of absorption from outside the emission-line region. If the last parameter is 1 then emergent intensities are reported. The values 2 and 3 are the equivalent quantities for the cumulative intensities in a time dependent model.

Sometimes the line label and wavelength are not enough to uniquely specify a line. For this case an alternate calling sequence can be used. The line can be disambiguated by specifying either the indices of the lower and upper level, or the energy of the lower level (see Section 2.5.3 in Hazy 1 for further details). When using *cdLine*, this can be done as follows:

```
#include "cddefines.h"
#include "cddrive.h"
#include "lines.h"
double relint, absint;
long nType = 0;

// example using lower and upper level index
if( cdLine( LineID("H  1", 46524.7_air, 11, 23), &relint, &absint, nType ) < 0 )
    printf("did not find this line\n");
// same line, but using lower level energy (in cm^-1) instead
if( cdLine( LineID("H  1", 46524.7_air, 105291.6), &relint, &absint, nType ) < 0 )
    printf("did not find this line\n");
```

If *cdLine* finds the line it returns the index of the line within the stack of emission lines. So a positive return value indicates success. It returns the negative of the total number of lines in the stack if the line is not found. This may occur if the line wavelength or label was mistyped. This is an exception to the C++ function return convention in which a normal return is zero and an abnormal return is non-zero. A positive value indicates a successful return.

There is a special version, *cdLine_ip*, which takes the line index as the first argument and return the relative and absolute intensities as the second and third quantities. The line index is not a constant for a given version of the code. It depends (amongst others) on the number of elements that are included, the sizes of the iso-sequence model atoms, and whether other models like H_2 are included.

8.6.13 cdnZone—how many zones in the last iteration?

The routine returns the number of zones in the previous iteration.

8.6.14 cdPressure_depth—pressure structure of the last iteration

The pressure as a function of depth, for the last iteration, is obtained by calling routine *cdPressure_depth*. This routine has three arguments, pointers to vectors giving the total pressure, the gas pressure, and the line radiation pressure. All are double precision vectors and the calling routine must have allocated space for these before calling the routine. The total number of

elements needed for each vector is the number of zones in the last iteration and is obtained by calling routine *cdnZone*.

8.6.15 cdPressure_last—pressure of the last zone

The pressure for the last zone is obtained by calling routine *cdPresure_last*. This routine has three arguments, pointers to the total pressure, the gas pressure, and the line radiation pressure. All are double precision variables. The total pressure includes all contributors to the pressure and may include magnetic, radiation, and turbulent pressure in addition to thermal pressure.

8.6.16 cdTemp—the computed mean temperature

There are two versions of the *cdTemp* function. Both return the mean electron temperature weighted with respect to some species.

cdTemp(element, stage, &Temp, weight)

This version supports all ions, the "H2" molecule, and a few special labels.

The first parameter is a four character null-terminated string giving the first four letters (upper or lower case) of the name of an element as spelled by the code. The second parameter is the ionization stage, with 1 for the atom, 2 the first ion, etc. The third parameter will be the computed mean temperature. The last parameter is a six-character null-terminated string, either "radius", "area", or "volume", that says whether the temperature should be weighted with respect to radius, area, or volume. These would be appropriate to compare to pencil beam observations, integrated long slit observations, or observations of the whole nebula, respectively. The mean temperature weighted by ion $+n$ of element S over radius is defined as

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(l)\, dl}{\int n(S^{+n})\, f(l)\, dl} \quad \text{[K]}, \tag{8.4}$$

the average over area is

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(r)\, r\, dr}{\int n(S^{+n})\, f(r)\, r\, dr} \quad \text{[K]}, \tag{8.5}$$

and the average over volume is

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(r)\, r^2\, dr}{\int n(S^{+n})\, f(r)\, r^2\, dr} \quad \text{[K]}. \tag{8.6}$$

The routine returns 0 if it finds the species, and 1 if it could not find the species. The following is an example of a call:

```
if( cdTemp("carb", 2, &temp, "radius") )
{
    cdEXIT(EXIT_FAILURE);
}
printf("The mean C+ temperature is %g\n", temp);
```

An ionization stage of zero requests one of the following special temperatures. All these can be weighted by radius, area, or volume.

21 cm-related temperatures: The routine will return one of three temperatures related to 21 cm observations. The label "***21cm***" will return the mean of $n(\mathrm{H}^0)/T_{kin}$, the harmonic mean gas kinetic temperature weighted with respect to the atomic hydrogen density. The label "**spin**" will return the mean weighted by $n(\mathrm{H}^0)/T_{spin}$, the harmonic mean of the 21 cm spin temperature weighted with respect to the atomic hydrogen density. Finally the label "**opti**" returns the temperature derived from the ratio of Lα to 21 cm optical depths (see AGN3 section 5.5).

Molecular hydrogen: The label "**H2**" and an ionization stage of zero will return the mean temperature weighted with respect to the H_2 density.

Simple mean temperature: If the label is an empty string, as in "", and the ionization stage is zero, the routine will return the mean temperature, but not weighted by any species. If the label is "**TeNe**" then the routine will return the mean temperature weighted by the electron density. If the label is shorter than four characters, padding the string with spaces is optional for backward compatibility[5].

cdTerm(species, &Temp, weight)

This version supports all ions, all molecules, and a few special labels.

The first parameter is the string of the ionic or molecular species. The second parameter will be the computed mean temperature. The last parameter is a six-character null-terminated string, either "radius", "area", or "volume", that says whether the temperature should be weighted with respect to radius, area, or volume. These would be appropriate to compare to pencil beam observations, integrated long slit observations, or observations of the whole nebula, respectively. The mean temperature weighted by ion $+n$ of element S over radius is defined as

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(l)\, dl}{\int n(S^{+n})\, f(l)\, dl} \quad [\mathrm{K}], \tag{8.7}$$

the average over area is

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(r)\, r\, dr}{\int n(S^{+n})\, f(r)\, r\, dr} \quad [\mathrm{K}], \tag{8.8}$$

and the average over volume is

$$\left\langle T\left(S^{+n}\right)\right\rangle = \frac{\int T\, n(S^{+n})\, f(r)\, r^2\, dr}{\int n(S^{+n})\, f(r)\, r^2\, dr} \quad [\mathrm{K}]. \tag{8.9}$$

The routine returns 0 if it finds the species, and 1 if it could not find the species. The following is an example of a call:

[5] In version C13 and before, the label string had to be exactly 4 characters long at all times.

```
if( cdTemp("C+", &temp, "radius") )
{
    cdEXIT(EXIT_FAILURE);
}
printf("The mean C+ temperature is %g\n", temp);
```

The following special temperatures are supported. All these can be weighted by radius, area, or volume.

21 cm-related temperatures: The routine will return one of three temperatures related to 21 cm observations. The label "***21cm***" will return the mean of $n(\mathrm{H}^0)/T_{kin}$, the harmonic mean gas kinetic temperature weighted with respect to the atomic hydrogen density. The label "**spin**" will return the mean weighted by $n(\mathrm{H}^0)/T_{spin}$, the harmonic mean of the 21 cm spin temperature weighted with respect to the atomic hydrogen density. Finally the label "**opti**" returns the temperature derived from the ratio of Lα to 21 cm optical depths (see AGN3 section 5.5).

Simple mean temperature: If the label is an empty string, as in "", the routine will return the mean temperature, but not weighted by any species. If the label is "**TeNe**" then the routine will return the mean temperature weighted by the electron density.

8.6.17 cdTemp_last—the temperature of the last zone

The kinetic temperature of the last zone is obtained by calling the function *cdLastTemp*. The function has no arguments and its return value is the temperature.

8.6.18 cdTimescales—several timescales.

This routine has three arguments, pointers to doubles that return the timescales [s] for several processes. These are the thermal timescale, the hydrogen recombination timescale, and the H_2 formation timescale.

8.7 Other information

8.7.1 cdDate(cdString)

The date when the current version of the code was released will be placed as a null-terminated string. The string is passed as an argument and the calling program must have allocated enough room for the string.

8.7.2 cdVersion(cdString)

The code's version number will be placed as a null-terminated string into the string passed as an argument. The version number is a string rather than a float since it can end with a letter of the alphabet. The calling program must allocate enough space for the string.

8.7.3 double cdExecTime()

This returns the time that has elapsed since the previous call to *cdInit*.

8.8 Printing comments

CLOUDY is designed to be autonomous and self aware. It constantly monitors itself to make sure that it is doing the physics correctly. After the calculation is complete, but before the emission lines are printed, it generates a series of statements that indicate warnings, cautions, comments, and surprises. These should be examined to confirm that the calculation is likely to be valid. A series of routines allows the driving code to determine whether these comments were generated, what type they were, and to print then into an arbitrary open file.

8.8.1 Were comments generated?

Routine *cdNwcns* will return the number of warnings, cautions, surprises, notes, and temperature and pressure failures:

```
cdNwcns( &lgAbort , &nw , &nc , &nn , &ns , &nte , &npe , &nione, &neden )
```

where the first variable is a *bool* flag indicating whether the calculation aborted, *nw* is the number of warnings generated (if this number is non-zero, then the calculation has serious problems), *nc* is the number of cautions generated (these are less severe than warnings, but are still a cause of concern), and *nn* and *ns* are the number of notes and surprises. The next two arguments are the number of temperature and pressure failures. The last two are the number of ionization and electron density failures. There should not be any failures in a successful calculation.

If either of the first two variables are non-zero then the code ran into serious problems. An abort is far more serious than a warning since it indicates catastrophic failure. I would appreciate learning about these. Please post details on the code's discussion board.

8.8.2 Printing the comments.

A series of comments normally appear after the last zone. These may be printed into any file by calling the series of subroutines described here. In all cases the routines take as an argument a file handle which must point to a file that has already been opened for writing.

```
/* output the comments into a file
 * first define the file handle, then open the file for writing */
FILE *ioOUT;
if( (IoOUT = fopen( "comments.txt", "w") ) == NULL )
{
    printf("error creating comments.txt file\n");
    cdEXIT(EXIT_FAILURE);
}
--- missing code to do calculation  ---
/*print the reason the calculation stopped, and geometry*/
cdReasonGeo(ioOUT);
/*print the warnings*/
```

```
cdWarnings(ioOUT);
/*next print the cautions*/
cdCautions(ioOUT);
/*now print any surprising results*/
cdSurprises(ioOUT);
/*now print the notes*/
cdNotes(ioOUT);
fclose(ioOUT);
```

cdReasonGeo(FILE *io) It is very important to understand why the calculation stopped. The first two lines after the last zone results give the reason the calculation stopped and the type of geometry. This information will be printed into the file whose handle is the argument.

cdWarnings(FILE *io) All warnings (denoted by "W-") will be printed.

cdCautions(FILE *io) All cautions (denoted by a "C-") will be printed.

cdSurprises(FILE *io) All surprises (denoted by a "!") are printed.

cdNotes(FILE *io) The notes concerning the calculation will be printed.

8.8.3 cdErrors(FILE *io)—printing a summary of any problems

Routine *cdErrors(FILE *io)* will generate a summary of any problems that happened during a calculation. The argument is a pointer to the output file where the summary will be placed. The calling program must have already opened the file for writing. If problems occurred in the calculation, such as temperature or pressure failures, warnings, or cautions, will be printed along with the calculation's title.

8.8.4 cdPrintCommands(FILE *io)—print the command stack

The entire series of input commands will be written into the file. The single argument is a file handle that points to a previously opened file. The commands are preceded and followed by lines that begin with "c =====" to easily identify their start and end.

8.8.5 setbuf or the no buffering command

Programs produce output by writing into a buffer. They only place information on the disk once the buffer is 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 C++ io library provides a routine, *setbuf*, that can turn file buffering off. The following sequence would open a file and turn buffering off:

```
ioDATA = open_data("test.out","w",AS_LOCAL_ONLY);
/* turn off buffering so we see results as then happen */
setbuf( ioDATA , NULL );
```

Note that the call to *setbuf must* come immediately after the call to *open_data* before any output is written. The **no buffering** command, described in Part 1 of this document, will do the same thing. Note that turning off buffering will make the code run far more slowly.

8.9 Example Call as a Subroutine

The file `template.cpp` shown below contains a skeleton program showing how you can call Cloudy as a subroutine. You can find the program in the directory `tsuite/programs`. Use this as a starting point to write your own program. The area where you can insert your own code is clearly indicated in the template.

```
/* This file is part of Cloudy and is copyright (C)1978-2025 by Gary J. Ferland and
 * others.  For conditions of distribution and use see copyright notice in license.txt */
/* Template main program for calling Cloudy as a subroutine
 * Routine returns 0 if model is ok, and 1 if problems occurred. */
#include "cddefines.h"
#include "cddrive.h"

int main( int argc, char *argv[] )
{
    exit_type exit_status = ES_SUCCESS;

    DEBUG_ENTRY( "main()" ); // do not remove this!

    try {
        // ========================================================================
        // START ENTERING YOUR CODE AFTER THIS LINE
        // inside this try block you can enter your code to call Cloudy as a subroutine
        // replace the code between here and the next ===== line with your own program

        // the code always needs to be initialized first
        cdInit();

        // to write output to a file, you MUST open it with open_data()
        // no need to check for a NULL pointer on return as open_data() will have done that already
        FILE* io = open_data("sample.out", "w");

        // you can call Cloudy in a loop if you want...
        for( int i=0; i < 1; ++i )
        {
            // the code always needs to be initialized first
            cdInit();
            // replace this with a series of calls to cdRead to define the input script
            // this particular command line exercises the smoke test
            cdRead( "test" );
            // this calls Cloudy to execute the input script you defined above
            if( cdDrive() )
                exit_status = ES_FAILURE;
        }

        cdEXIT(exit_status); // always exit with cdEXIT, this assures files are properly closed.
        // ========================================================================
        // THIS IS THE END OF THE PROGRAM YOU WROTE
        // this ends the try block - your code calling Cloudy ends above this line
    }
    // here we catch all the possible exceptions that the code can throw, do not remove this!
    catch( bad_alloc )
    {
        fprintf( ioQQQ, " DISASTER - A memory allocation has failed. Most likely your computer "
             "ran out of memory.\n Try monitoring the memory use of your run. Bailing out...\n" );
        exit_status = ES_BAD_ALLOC;
    }
    catch( out_of_range& e )
    {
        fprintf( ioQQQ, " DISASTER - An out_of_range exception was caught, what() = %s. Bailing out...\n",
             e.what() );
        exit_status = ES_OUT_OF_RANGE;
    }
    catch( domain_error& e )
    {
        fprintf( ioQQQ, " DISASTER - A vectorized math routine threw a domain_error. Bailing out...\n" );
        fprintf( ioQQQ, " What() = %s", e.what() );
        exit_status = ES_DOMAIN_ERROR;
    }
    catch( bad_assert& e )
    {
        MyAssert( e.file(), e.line() , e.comment() );
        exit_status = ES_BAD_ASSERT;
    }
    catch( bad_signal& e )
    {
        if( e.sig() == SIGILL )
        {
            if( ioQQQ != NULL )
                fprintf( ioQQQ, " DISASTER - An illegal instruction was found. Bailing out...\n" );
            exit_status = ES_ILLEGAL_INSTRUCTION;
        }
        else if( e.sig() == SIGFPE )
        {
            if( ioQQQ != NULL )
                fprintf( ioQQQ, " DISASTER - A floating point exception occurred. Bailing out...\n" );
```

```
            exit_status = ES_FP_EXCEPTION;
        }
        else if( e.sig() == SIGSEGV )
        {
            if( ioQQQ != NULL )
                fprintf( ioQQQ, " DISASTER - A segmentation violation occurred. Bailing out...\n" );
            exit_status = ES_SEGFAULT;
        }
#       ifdef SIGBUS
        else if( e.sig() == SIGBUS )
        {
            if( ioQQQ != NULL )
                fprintf( ioQQQ, " DISASTER - A bus error occurred. Bailing out...\n" );
            exit_status = ES_BUS_ERROR;
        }
#       endif
        else
        {
            if( ioQQQ != NULL )
                fprintf( ioQQQ, " DISASTER - A signal %d was caught. Bailing out...\n", e.sig() );
            exit_status = ES_UNKNOWN_SIGNAL;
        }
    }
    catch( cloudy_abort& e )
    {
        fprintf( ioQQQ, " ABORT DISASTER PROBLEM - Cloudy aborted, reason: %s\n", e.comment() );
        exit_status = ES_CLOUDY_ABORT;
    }
    catch( cloudy_exit& e )
    {
        if( ioQQQ != NULL )
        {
            ostringstream oss;
            oss << " [Stop in " << e.routine();
            oss << " at " << e.file() << ":" << e.line();
            if( e.exit_status() == 0 )
                oss << ", Cloudy exited OK]";
            else
                oss << ", something went wrong]";
            fprintf( ioQQQ, "%s\n", oss.str().c_str() );
        }
        exit_status = e.exit_status();
    }
    catch( std::exception& e )
    {
        fprintf( ioQQQ, " DISASTER - An unknown exception was caught, what() = %s. Bailing out...\n",
             e.what() );
        exit_status = ES_UNKNOWN_EXCEPTION;
    }
    // generic catch-all in case we forget any specific exception above... so this MUST be the last one.
    catch( ... )
    {
        fprintf( ioQQQ, " DISASTER - An unknown exception was caught. Bailing out...\n" );
        exit_status = ES_UNKNOWN_EXCEPTION;
    }

    cdPrepareExit(exit_status);

    return exit_status;
}
```

8.10 Computing Grids of Calculations

Today I usually use the code to compute results, extract information, and save desired quantities. The following example illustrates producing a series of models with increasing gas temperature and density. The program calculates the line strength of various diagnostic [O III] lines normalized to [O III] λ5007 and writes these to a file. This example is the program `vary_nete.cpp`, which you can find in the directory `tsuite/programs/vary_nete`.

This example only saves results for a few lines. Often a large number of lines are needed. A call to *cdLineList* provides an easy way to obtain large numbers of lines whose labels are stored in a file.

```
/* This file is part of Cloudy and is copyright (C)1978-2025 by Gary J. Ferland and
 * others.  For conditions of distribution and use see copyright notice in license.txt */
/*main program that calls cloudy when used as a stand-alone program */
#include "cddefines.h"
#include "cddrive.h"

/*int main( int argc, char *argv[] )*/
```

```
int main( void )
{
    exit_type exit_status = ES_SUCCESS;

    DEBUG_ENTRY( "main()" );

    try {
        double hdenLimit , hdenInit , hden, TeInc ,
            r5007,r4363,r1665,ro3_88,ro3_52, r1661 ,
            absolute , temp, TeLimit, TeInit , hdenInc;

        FILE *ioDATA ;
        char chLine[100];

        /* initialize the code for this run */
        cdInit();

        cdOutput( "vary_nete.out" );

        /* calculation's results will go to this file*/
        ioDATA = open_data("vary_nete.txt","w");

        /* the range of density, and the increment in density, for this grid */
        hdenInit = 0.;
        hdenLimit = 7.;
        hdenInc = 1.;

        /* the range of log temperatures for the grid */
        TeInit = 3.5;
        TeLimit = 4.5;
        /* multiplicative inc - log */
        TeInc = .2;

        /* set the density and temperature to the initial values */
        hden = hdenInit;
        temp = TeInit;

        /* print the header for the data file */
        fprintf(ioDATA,
            "density\ttemp\t[O III] 5007\t[O III] 4363\t[O III] 1665\t[O III] 88\t[O III] 52\t[O III] 1661\n");

        while( hden < 1.01 * hdenLimit )
        {
            while( temp < 1.01*TeLimit )
            {
                /* initialize the code for this run */
                cdInit();

                /* option to not execute the code, uncomment when debugging setup */
                /*cdNoexec( );*/

                /* gas temperature for this calculation */
                sprintf(chLine,"constant temperature %f", temp);
                cdRead( chLine );

                /* gas density for this calculation */
                sprintf(chLine,"hden %f", hden);
                cdRead( chLine );

                /* only want the first zone */
                cdRead( "stop zone 1" );

                /* speed up calculation by not included some elements and lines */
                cdRead( "init file \"fast.ini\"" );

                cdRead( "normalize to \"o  3\" 5006.84" );

                /* an incident continuum must be specified to get the code
                 * to run at all - not very important since we will set
                 * the gas temperature */
                cdRead( "blackbody 40000" );
                cdRead( "ionization parameter -3" );

                /* actually call the code */
                if( cdDrive() )
                    exit_status = ES_FAILURE;
                /* flush the output so we see it on the screen */
                fflush(ioQQQ);

                fprintf(ioDATA,"%.3e\t%.5f",    hden, temp );
                fprintf(stderr,"%.3e\t%.5f",    hden, temp );

                /********************** O III ******************/
                if( cdLine( "O  3", 5006.84_air, &r5007 , &absolute ) < 0 )
                {
                    printf("did not find O  3 5007\n");
                    exit_status = ES_FAILURE;
                }
                /* this should be unity */
                fprintf(ioDATA,"\t%.3e",    r5007 );
                fprintf(stderr,"\t%.3e",    r5007 );
```

```
                if( cdLine( "O  3", 4363.21_air, &r4363 , &absolute ) < 0 )
                {
                    printf("did not find totl 4363\n");
                    exit_status = ES_FAILURE;
                }
                fprintf(ioDATA,"\t%.3e",    r4363 );
                fprintf(stderr,"\t%.3e",    r4363 );

                if( cdLine( "blnd", 1666._vac, &r1665 , &absolute ) < 0 )
                {
                    printf("did not find totl 1665\n");
                    exit_status = ES_FAILURE;
                }
                fprintf(ioDATA,"\t%.3e",    r1665 );
                fprintf(stderr,"\t%.3e",    r1665 );

                if( cdLine( "O  3", 883323._air, &ro3_88 , &absolute ) < 0 )
                {
                    printf("did not find O  3 88\n");
                    exit_status = ES_FAILURE;
                }
                fprintf(ioDATA,"\t%.3e",    ro3_88 );
                fprintf(stderr,"\t%.3e",    ro3_88 );

                if( cdLine( "O  3", 518004._air, &ro3_52 , &absolute ) < 0 )
                {
                    printf("did not find O  3 52\n");
                    exit_status = ES_FAILURE;
                }
                fprintf(ioDATA,"\t%.3e",    ro3_52 );
                fprintf(stderr,"\t%.3e",    ro3_52 );

                if( cdLine( "O  3", 1660.81_vac, &r1661 , &absolute ) < 0 )
                {
                    printf("did not find O  3 1661\n");
                    exit_status = ES_FAILURE;
                }
                fprintf(ioDATA,"\t%.3e",    r1661 );
                fprintf(stderr,"\t%.3e",    r1661 );


                /************************ end lines with lf and flush it ***************/
                fprintf(ioDATA,"\n" );
                fflush(ioDATA );
                fprintf(stderr,"\n" );

                temp += TeInc;
            }
            temp = TeInit;
            hden += hdenInc;
        }

        cdEXIT(exit_status);
    }
    catch( bad_alloc& )
    {
        fprintf( ioQQQ, " DISASTER - A memory allocation has failed. Most likely your computer "
             "ran out of memory.\n Try monitoring the memory use of your run. Bailing out...\n" );
        exit_status = ES_BAD_ALLOC;
    }
    catch( out_of_range& e )
    {
        fprintf( ioQQQ, " DISASTER - An out_of_range exception was caught, what() = %s. Bailing out...\n",
             e.what() );
        exit_status = ES_OUT_OF_RANGE;
    }
    catch( domain_error& e )
    {
        fprintf( ioQQQ, " DISASTER - A vectorized math routine threw a domain_error. Bailing out...\n" );
        fprintf( ioQQQ, " What() = %s", e.what() );
        exit_status = ES_DOMAIN_ERROR;
    }
    catch( bad_assert& e )
    {
        MyAssert( e.file(), e.line() , e.comment() );
        exit_status = ES_BAD_ASSERT;
    }
#ifdef CATCH_SIGNAL
    catch( bad_signal& e )
    {
        if( ioQQQ != NULL )
        {
            if( e.sig() == SIGINT || e.sig() == SIGQUIT )
            {
                fprintf( ioQQQ, " User interrupt request. Bailing out...\n" );
                exit_status = ES_USER_INTERRUPT;
            }
            else if( e.sig() == SIGTERM )
            {
                fprintf( ioQQQ, " Termination request. Bailing out...\n" );
                exit_status = ES_TERMINATION_REQUEST;
            }
```

```
            else if( e.sig() == SIGILL )
            {
                fprintf( ioQQQ, " DISASTER - An illegal instruction was found. Bailing out...\n" );
                exit_status = ES_ILLEGAL_INSTRUCTION;
            }
            else if( e.sig() == SIGFPE )
            {
                fprintf( ioQQQ, " DISASTER - A floating point exception occurred. Bailing out...\n" );
                exit_status = ES_FP_EXCEPTION;
            }
            else if( e.sig() == SIGSEGV )
            {
                fprintf( ioQQQ, " DISASTER - A segmentation violation occurred. Bailing out...\n" );
                exit_status = ES_SEGFAULT;
            }
#           ifdef SIGBUS
            else if( e.sig() == SIGBUS )
            {
                fprintf( ioQQQ, " DISASTER - A bus error occurred. Bailing out...\n" );
                exit_status = ES_BUS_ERROR;
            }
#           endif
            else
            {
                fprintf( ioQQQ, " DISASTER - A signal %d was caught. Bailing out...\n", e.sig() );
                exit_status = ES_UNKNOWN_SIGNAL;
            }

        }
    }
#endif
    catch( cloudy_exit& e )
    {
        if( ioQQQ != NULL )
        {
            ostringstream oss;
            oss << " [Stop in " << e.routine();
            oss << " at " << e.file() << ":" << e.line();
            if( e.exit_status() == 0 )
                oss << ", Cloudy exited OK]";
            else
                oss << ", something went wrong]";
            fprintf( ioQQQ, "%s\n", oss.str().c_str() );
        }
        exit_status = e.exit_status();
    }
    catch( std::exception& e )
    {
        fprintf( ioQQQ, " DISASTER - An unknown exception was caught, what() = %s. Bailing out...\n",
             e.what() );
        exit_status = ES_UNKNOWN_EXCEPTION;
    }
    // generic catch-all in case we forget any specific exception above... so this MUST be the last one.
    catch( ... )
    {
        fprintf( ioQQQ, " DISASTER - An unknown exception was caught. Bailing out...\n" );
        exit_status = ES_UNKNOWN_EXCEPTION;
    }

    cdPrepareExit(exit_status);

    return exit_status;
}
```

Chapter 9

THE EMISSION LINES

9.1 Overview

The following sections outline the emission lines predicted by CLOUDY. Before version 90 of the code all lines were listed in the sub-section immediately following this section. The code is being modified to bring all lines into a common line class, as the code moves to C++ and objects. This chapter will remain incomplete until this work is finished.

9.2 The main emission-line printout

The main emission line printout was briefly described in the Chapter *OUTPUT*. This section goes into more detail.

Output organization. The printed list is sorted into four large groups of columns, with each large column sub-divided into four smaller sub-columns. The first sub-column is either the spectroscopic designation of the ion producing the line or an indication of how the line is formed. The second sub-column is the line wavelength, with a 0 to indicate a continuum. The third sub-column is the log of the power in the line, in the units given in the header (erg s^{-1} into either 4π sr or cm^{-2}). The last sub-column is the intensity of the line relative to the reference line, usually Hβ , unless this is reset with the **normalize** command.

These lines can be printed as a single large column, and can be sorted by wavelength or intensity. These options are controlled by the **print line** command described in Part I of this document.

9.2.1 Intrinsic and emergent line intensities

See Section 2.10.

9.2.2 Units of Line wavelengths

These can be given in various units. Numbers ending in "A" are wavelengths in angstrom (Å). For instance, Hβ is given by "H 1 4861.32A". Wavelengths in micron are indicated by "m", an example, the strong [O III] IR line, is "O 3 51.8004m".

Continua are usually indicated by a wavelength of zero.

9.2.3 Air vs vacuum wavelengths

The emission line wavelengths follow the convention that vacuum wavelengths are used for $\lambda_{\rm vac} \leq 2000$ Å and STP air wavelengths are used for $\lambda_{\rm vac} > 2000$ Å. The **print line vacuum** command tells the code use use vacuum wavelengths throughout. **Save continuum** output is always reported in vacuum wavelengths to avoid a discontinuity at 2000 Å.

9.2.4 Blocks of lines in main output

Lines are organized by common origin with a comment, ending in a series of periods "...", beginning the section. As an example, the first commented block of lines begins with "general properties...". The following subsections give overviews of the lines.

9.2.5 General properties...

This mainly summarizes heating and cooling agents for the model.

H 1 4861 and H 1 1216, are the total intensities of Hβ and Lα, as predicted by the multi-level H atom. These intensities are the results of calculations that include all collisional, radiative, and optical depth effects.

Inci The total energy in the incident continuum. This entry will not be included if the **aperture** command is in effect.

TotH and TotC give the total heating and cooling. These will be nearly equal in equilibrium.

BFH1 and BFHx are the heating due to photoionization of ground state and excited state hydrogen respectively.

He1i, 3He1 , heating due to ground state He and the triplets.

BFHe and TotM are the heating due to helium and metal photoionization.

Pair heating due to pair production.

ComH , ComC , Compton heating, cooling.

CT H CT C charge transfer heating and cooling.

extH extC "extra" heating or cooling added to model.

e-e+ 511 The positron line.

Expn , expansion, or adiabatic, cooling

H FB , H radiative recombination cooling

HFBc, HFBc , hydrogen net free-bound cooling and heating

Iind , cooling due to induced recombination of hydrogen

3He2 , cooling due to induced recombination of fully ionized helium

Cycn , cyclotron cooling

9.2.6 Continua...

These give intensities of various continua. These are either the total integrated continuum or the product νF_ν at certain energies.

Continuum bands

The file `continuum_bands.dat` in the data directory specifies a set of wavelength bands. The code will integrate over these bands to find the total radiated luminosity and enter this into the main emission-line stack. Currently this is a simple sum of the energy emitted between the upper and lower bounds of the band, and does not take into account the transmission function of particular instruments. The `continuum_bands.dat` file can be edited to change the number of bands or their detailed properties. Table 9.1 lists the bands in the file at the time of this writing. The first and second columns give the label and wavelength as they appear in the printout. The last column gives the wavelength range for the integration. The first wavelength is treated as a label and will always appear in the output as shown in the table. The last two numbers are interpreted as vacuum wavelengths. These entries will not be included if the **aperture** command is in effect. Please consult the file to see its current contents and feel free to add your own bands.

Other continua

Bac 3646 residual flux at head of Balmer continuum, νF_ν. This entry will not be included if the **aperture** command is in effect.

cout 3646 cref 3646 , outward, reflected continuum at peak of Balmer Jump. These entries will not be included if the **aperture** command is in effect.

thin 3646 , residual flux at head of Balmer continuum, optically thin limit. This entry will not be included if the **aperture** command is in effect.

Inci 4860, Inci 1215 , incident continua near Hα and Lα. These entries will not be included if the **aperture** command is in effect.

Ba C 0 , integrated Balmer continuum

PA C 0 , integrated Paschen continuum

HeFF 0 , He brems emission

HeFB 0 , He recombination cooling

MeFB 0 , heavy element recombination cooling

Table 9.1: Default continuum bands

Label	Wavelength	Wavelength Range
FIR	83.0000m	40.0000m – 500.000m
TIR	1800.00m	500.000m – 3100.00m
NIRa	2.85000m	7000.00A – 40.0000m
NIRb	3.00000m	10000.0A – 5.00000m
MIRa	15.0000m	5.00000m – 25.0000m
MIRb	22.5000m	5.00000m – 40.0000m
NMIR	21.7500m	7000.00A – 40.0000m
TFIR	611.250m	122.500m – 1100.00m
TALL	10000.0A	0.0100000A – 10000.0m
F12	12.0000m	8.50000m – 15.0000m
F25	25.0000m	19.0000m – 30.0000m
F60	60.0000m	40.0000m – 80.0000m
F100	100.000m	83.0000m – 120.000m
MIPS	24.0000m	20.8000m – 26.1000m
MIPS	70.0000m	61.0000m – 80.0000m
MIPS	160.000m	140.000m – 174.000m
IRAC	3.60000m	3.16000m – 3.92000m
IRAC	4.50000m	4.00000m – 5.02000m
IRAC	5.80000m	5.00000m – 6.40000m
IRAC	8.00000m	6.50000m – 9.30000m
SPR1	250.000m	212.000m – 288.000m
SPR2	350.000m	297.000m – 405.000m
SPR3	500.000m	414.000m – 600.000m
PAC1	70.0000m	60.0000m – 82.0000m
PAC2	100.000m	84.0000m – 122.000m
PAC3	160.000m	130.000m – 198.000m
PAH	3.30000m	3.25000m – 3.35000m
PAHC	3.23000m	3.20000m – 3.25000m
PAHC	3.37000m	3.35000m – 3.40000m
PAH	6.20000m	5.90000m – 6.40000m
PAHC	5.65000m	5.40000m – 5.90000m
PAH	7.90000m	7.40000m – 8.40000m
PAHC	6.90000m	6.40000m – 7.40000m
PAH	11.3000m	11.1000m – 11.5000m
PAHC	10.9000m	10.7000m – 11.1000m
PAH	11.8000m	11.6000m – 12.3000m
PAHC	12.6500m	12.3000m – 13.0000m
PAH	13.3000m	12.9000m – 13.7000m
PAHC	14.1000m	13.7000m – 14.5000m
Bcon	3640.00A	911.600A – 3646.40A
Pcon	5000.00A	3646.40A – 8204.40A
O3bn	5007.00A	4980.00A – 5100.00A
SX	25.0000A	8.26000A – 41.3000A
HX	4.70000A	1.23000A – 8.26000A
ROSA	12.3980A	5.16600A – 123.980A

MeFF 0 , metal brems emission

ToFF 0 , total brems emission

FF x , part of H brems, in x-ray beyond 0.5KeV

eeff , electron - electron brems

nFnu 122m, ***nInu 122m***, ***InwT 122m***, ***InwC 122m***, a large list of continua at selected wavelengths will be printed. These entries will not be included if the **aperture** command is in effect. The first is the sum of various continua at the wavelength, given as νF_ν (see the **set nFnu** command in Part 1 for a discussion of what is included in the ***nFnu*** entry). ***nInu*** is the transmitted and reflected incident continuum. ***InwT*** is the total reflected continuum. ***InwC*** is the reflected incident continuum.

9.2.7 Molecules...

H2dC , is the cooling due to collisional dissociation of H_2.

H2dH , heating by H_2 dissociation by Lyman continuum

H2vH , heating by coll deexcit of vib-excited H_2

H2vC , cooling by coll deexcit of vib-excited H_2

H2 v , line emission by vib-excited H_2

H-FB and H-FF are the free-bound and free-free continua of the H- ion.

H-CT 6563 , H-alpha produce by H- mutual neutralization

H- H 0, H- heating

H-Hc 0, H- heating

H2+ and HEH+ are the cooling due to formation of H_2^+ and HeH^+.

Codh , carbon monoxide photodissociation heating

CO C 12 , C12O16 cooling

CO C 13 , C13O16 cooling

9.2.8 Species Bands...

Bands in which the emission of a certain species is accumulated are reported in the section of block of lines on the main output headlined with "`bands....`". User-specified bands may be provided with the **save species bands** command, described in Hazy 1, Section 16.86.1. By default, the Fe II bands defined in `data/FeII_bands.dat`, if iron is enabled in the model, even if not specified with such a command.

Note that these bands are more fully explained in the output of the command **save line labels**, see Hazy 1, Section 16.68.6.

9.2.9 Grains...

Information in this block concerns emission, absorption, heating, and cooling by any grains included in the calculation.

GrGH , gas heating by grain photoionization

GrTH , gas heating by thermionic emissions of grains

GrGC , gas cooling by collisions with grains

GraT , This is the total grain heating by all sources, lines, collisions, incident continuum. If the grain emission is optically thin limit then this is equal to the total intensity in grain emission.

GraI , grain heating by incident continuum

GraL 1216 , grain heating due to destruction of Lα

GraC , grain heating due to collisions with gas

GraD , grain heating due to diffuse fields, may also have grain emission

Grain emission is included in the predicted total emitted continuum. A machine readable form of the continuum can be produced with the **save continuum** command, also described in Part I of this document.

9.2.10 H-like iso-seq...

This block includes all hydrogen-like isoelectronic species. The **atom H-like** command, described in Part 1 of this document, adjusts properties of this sequence.

HFFc 0 , net free-free cooling, nearly cancels with cooling in lte

HFFh 0 , net free-free heating, nearly cancels with cooling in lte

H FF 0 , H brems (free-free) cooling

FF H 0 , total free-free heating

Clin 912 , total collisional cooling due to all hydrogen lines

Hlin 912 , total collisional heating due to all hydrogen lines

Cool 1215.67 , collisionally excited La cooling

Heat 1215.67 , collisionally de-excited La heating

Crst 960 , cooling due to n¿2 Lyman lines

Hrst 960 , heating due to n¿2 Lyman lines

Crst 4861.32 , cooling due to n¿3 Balmer lines

Hrst 4861.32 , heating due to n¿3 Balmer lines

Crst 0 , cooling due to higher Paschen lines

Hrst 0 , heating due to higher Paschen lines

LA X 1215.67 , Lα contribution from suprathermal secondaries from ground

Ind2 1215.67 , Lα produced by induced two photon

Pump 4861.32 , Hβ produced by continuum pumping in optically thin ld limit

CION 0 , net col ionz-3 body heat collision ionization cooling of hydrogen

3bHt 0 , heating due to 3-body recombination

Strk 1215.67 , Stark broadening component of line

Dest 1215.67 , part of line destroyed by background opacities

Fe 2 1215.67 , part of Lα absorbed by Fe II

Q(H) 4861.32 is the intensity of Hβ predicted from the total number of ionizing photons, Q(H^0), assuming that each hydrogen-ionizing photon produces one hydrogen atom recombination. This entry will not be included if the **aperture** command is in effect.

Q(H) 1215.67 indicates the Lα intensity produced if each hydrogen ionizing photon results in one Lα photon in the high density limit (i.e., no two-photon emission). This entry will not be included if the **aperture** command is in effect.

CaBo 4861.32 These are the "old" case B predictions, as printed in versions 90 and before of the code.

Ca B 6562.80A The entries starting with "Ca B" are the Case B intensities computed from the actual model ionization and temperature structure, but assuming that Hβ emits with its Case B emissivity.

Next the predicted intensities of all lines of the hydrogenic iso-electronic sequence are given. The lines have labels that identify the species and stage of ionization, such as "H 1", "He 2", "Li 3", "C 6", etc. The entries with double the wavelength of the Lyα line are the total intensities of the $2s-1s$ two-photon emission. The M1 line between these two levels is also reported and has a wavelength that is very close to the $2p_{1/2}-1s_{1/2}$ line. To discriminate it from the latter, "M1" is added to the line label. For light elements the two-photon emission is the dominant transition between these two levels, but for heavy elements the M1 line dominates.

9.2.11 He iso-sequence...

Atoms and ions of the helium-like iso-electronic sequence are treated as multi-level atoms. All species and stages of ionization are specified by labels like "He 1", "Li 2", "C 5", etc. The wavelength of the two-photon continuum $1s.2s\ ^1S_0 - 1s^2\ ^1S_0$ is reported as twice the wavelength derived from the energy difference between the two levels. The $2\ ^3P$ term is resolved into three levels. Emission of each line of the $2\ ^3S - 2\ ^3P$ and $1\ ^1S - 2\ ^3P$ multiplets is predicted along with the sum of the multiplets with label "Blnd". The **atom He-like** command, described in Part 1 of this document, adjusts properties of this sequence. Further details are given in Bauman et al. (2005), Porter et al. (2005), and Porter and Ferland (2007).

9.2.12 Recombination...

These are a set of heavy-element recombination lines that are predicted in the low-density limit assuming that the transitions are optically thin. This consists of all recombination lines of C, N., and O, with coefficients taken from Nussbaumer and Storey (1984) and Pequignot et al. (1991).

These predictions are for optically thin pure recombination. These should be accurate for planetary nebulae and H II regions. They will not be accurate for dense environments where optical depths and collisional effects come into play. These are only included in the output if the electron density is less than $10^8\,\mathrm{cm}^{-3}$, a rough upper limit to the range of validity in the original calculations of the coefficients.

There are several instances where more than one line of an ion will have the same wavelength.

9.2.13 Level 2 lines...

These are resonance lines that use Opacity Project wavelengths, which are generally accurate to about 10%. These lines have g-bar collision strengths, which are not very accurate at all.

9.3 The transferred lines

9.3.1 Save line data output

The group of "transferred lines" includes all those that have been moved to the `EmLine` class.

In older versions of this document a large list of emission lines appeared here. This list is now far too large to include here. Rather, the list can be generated by executing the code with the command **save line data "filename.txt"** included. This will create a file that includes the full set of lines that are predicted. Note that the lines that are output are only those that exist when the code is run. It is possible to make many of the model atoms and molecules as large or small as you like, and the actual lines that exist when the **save** command is entered will be output. The test case `func_lines.in` in the test suite includes this save command and generates a list of all transferred lines in the file `func_lines.lis`.

To generate a line list, set up a calculation with the atoms set to whatever size is desired (see the **atom** command in Part I). Then execute this script with the **save line data** command included (described in Part I). The save output will include the line list. This will include the level 2, H and

He iso-sequence, H_2, CO, and recombination lines, but not the scalar forbidden lines. These are described in a list following this subsection.

This contains several groups of lines. All quantities were evaluated at 10^4 K. The description of the command in Part I of this document explains how to evaluate the quantities at other temperatures.

The ion is the first column of the table. This is in a uniform format, beginning with the two character element symbol and followed by an integer indicating the level of ionization. "C 2" is C^+ or C II. This is followed by the wavelength used to identify the line in the printout. The third column, with the label "WL", is the correct wavelength of the line, with units of micron ("m"), angstrom ("A"), or centimeter ("c"). The remaining columns give the statistical weights of the lower and upper levels, the product of the statistical weight and the oscillator strength, and then the transition probability.

The last column is the electron collision strength. Usually these collision strengths are for only the indicated transition, although in some cases (the Be sequence) the value is for the entire multiplet.

9.3.2 Output produced for the transferred lines

Because the lines have a common format within their storage vectors, the output has a common format too. Generally only the total intensity of the transition, the result of the solution of a multi-level atom with all processes included, is printed. The approach used to compute the level populations is described in Part II of HAZY, and includes continuum pumping, destruction by background opacities, and trapping.

The total intensity of the transition is printed in a form like "C 2 1335", with the spectroscopic identification given by the first part, as found in the first column of the table, and the wavelength as indicated by the number in the second column of the table.

In a few cases (for instance, the C IV $\lambda\lambda$1548, 1551 doublet), a total intensity is also derived. In these cases the label "Blnd" will appear together with an average wavelength (1549 in this case). These lines are all explicitly shown in a following section.

It is possible to break out various contributors to the lines with options on the **print line** command, described in Part I of this document and in the following. These contributors are printed following the total intensity.

print line heating An emission line will heat rather than cool the gas if it is radiatively excited but collisionally de-excited. The print out will include this agent, with the label "Heat", when this command is given.

print line collisions The collisional contribution to the lines will be printed, with the label "Coll".

print line pump The contribution to the total line, produced by continuum pumping, is printed with the label "Pump". What is observed? Whether or not this is a net emission process contributing to the observed line intensity depends on the geometry, mainly whether or not continuum source is in the beam. At some velocities within the line profile this can be a net emission process, due to absorption at other velocities. If the continuum source is in the beam and gas covers it, this is not a net emission process, since photons are conserved.

print line inward The inwardly directed part of the total emission is printed with the label "Inwd". This can be greater than half of the line intensity if the line is optically thick since these

Table 9.2: Hydrogen emission lines

Series	$n' \rightarrow n$	Wavelength	I(Case B)
Lyman	2–1	1215.68A	-
Balmer Hα	3–2	6562.85A	2.8463
Hβ	4–2	4861.36A	1.0000
Hγ	5–2	4340.49A	0.4692
Hδ	6–2	4101.76A	0.2596
Paschen Pα	4–3	1.87511m	0.3319
Pβ	5–3	1.28181m	0.1617
Pγ	6–3	1.09381m	0.0899
Pδ	7–3	1.00494m	0.0553
Brackett Brα	5–4	4.05116m	0.0778
Brβ	6–4	2.62515m	0.0445
Brγ	7–4	2.16553m	0.0274
Brδ	8–4	1.94456m	0.0180
Pfund	6–5	7.45781m	0.0246
Humphreys	7–6	12.3685m	0.0098
	8–7	19.0566m	0.0042
	9–8	27.7957m	0.0020

lines tend to be radiated from the hotter illuminated face of the cloud.

print line optical depths At the end of the calculation the optical depths for all optically thick lines will be printed. This is not done by default since it can be quite long.

9.4 Line identifications

The file `line_labels.txt` in the docs directory of the distribution lists line identifications and a brief description of its origin.

9.5 Hydrogen recombination lines

Table 9.2 gives the strongest lines of the lowest series. All lines have the label "H 1". The wavelength column gives the string as it appears in the printout. "m" indicates a wavelength in μm and A in angstrom. The Case B intensity is taken from the `limit_caseb_h_hs87` test case.

Some lines may have the same wavelength if the default line precision is used. The **set line precision** command can be used to increase the number of significant figures in the line wavelength, which should make identification easier.

9.6 Molecular hydrogen lines

Table 9.3 gives some of the stronger or more frequently observed H_2 lines. These are only predicted when the large model H_2 molecule is included with the **atom H2** command. The

wavelength column gives the string as it appears in the printout. “m” indicated a wavelength in μm. All lines have the label “H2 ”.

Many lines will have the same wavelength if the default line precision is used. The **set line precision** command can be used to increase the number of significant figures in the line wavelength, which should make identification easier.

The following is an example which predicts the emissivity of the H_2 2.121 1-0 S(1) μm line.

```
save line emissivity ``lines.ems''
H2   2.121m
end of lines
```

A list of all H2 lines with their labels and excitation energies can be generated with the command **save H2 lines**. The Joint Astronomy Centre in Hawaii give a summary of H_2 lines.

9.7 CO lines

Rotation transitions within the ground vibration level are included. These are listed in Table 9.4 which gives the symbol “m” to indicate μm.

Table 9.3: Molecular hydrogen emission lines

Transition	v_{hi}, J_{hi}	v_{lo}, J_{lo}	λ(label)	χ(hi, K)
0-0 S(0)	0,2	0,0	28.2130m	509.8
0-0 S(1)	0,3	0,1	17.0300m	1015.1
0-0 S(2)	0,4	0,2	12.2752m	1681.6
0-0 S(3)	0,5	0,3	9.66228m	2503.8
0-0 S(4)	0,6	0,4	8.02362m	3474.3
0-0 S(5)	0,7	0,5	6.90725m	4586.2
0-0 S(6)	0,8	0,6	6.10718m	5829.5
1-0 O(2)	1,0	0,2	2.62608m	5986.9
1-0 Q(1)	1,1	0,1	2.40594m	6149.0
1-0 O(3)	1,1	0,3	2.80176m	6149.0
1-0 S(0)	1,2	0,0	2.22269m	6471.4
1-0 Q(2)	1,2	0,2	2.41307m	6471.4
1-0 O(4)	1,2	0,4	3.00305m	6471.4
1-0 S(1)	1,3	0,1	2.12125m	6951.3
1-0 Q(3)	1,3	0,3	2.42307m	6951.3
1-0 O(5)	1,3	0,5	3.23411m	6951.3
0-0 S(7)	0,9	0,7	5.50996m	7196.7
1-0 S(2)	1,4	0,2	2.03320m	7584.3
1-0 Q(4)	1,4	0,4	2.43683m	7584.3
1-0 O(6)	1,4	0,6	3.50043m	7584.3
1-0 S(3)	1,5	0,3	1.95702m	8365.0
1-0 Q(5)	1,5	0,5	2.45408m	8365.0
1-0 O(7)	1,5	0,7	3.80648m	8365.0
0-0 S(8)	0,10	0,8	5.05148m	8677.0
1-0 S(4)	1,6	0,4	1.89145m	9286.3
1-0 Q(6)	1,6	0,6	2.47510m	9286.3
0-0 S(9)	0,11	0,9	4.69342m	10261
1-0 S(5)	1,7	0,5	1.83529m	10341
1-0 S(6)	1,8	0,6	1.78746m	11521
1-0 S(7)	1,9	0,7	1.74760m	12817

Table 9.4: CO emission lines

Label	wavelength
CO	2600.05m
CO	1300.05m
CO	866.727m
CO	650.074m
CO	520.089m
CO	433.438m
CO	371.549m
CO	325.137m
CO	289.041m
CO	260.169m
CO	236.549m
CO	216.868m
CO	200.218m
CO	185.949m
CO	173.584m
CO	162.767m
CO	153.225m
CO	144.745m
CO	137.159m
CO	130.333m
CO	124.160m
CO	118.548m
CO	113.427m
CO	108.733m
CO	104.416m
CO	100.433m
CO	96.7462m
CO	93.3237m
CO	90.1384m
CO	87.1666m
CO	84.3877m
CO	81.7835m
CO	79.3383m
CO	77.0375m
CO	74.8697m
CO	72.8231m
CO	70.8878m
CO	69.0557m
CO	67.3181m
CO	65.6684m

Chapter 10

PROBLEMS

10.1 Introduction

The code is designed to be autonomous and self-aware. Nonetheless, if can run into problems. This section describes some of the errors that can cause CLOUDY to stop. Floating point errors should never occur. Several other internal errors, which the code is designed to trap and then complain about, could occur. Finally, it is possible that the code will stop because of convergence problems.

The most important single thing to understand about any calculation is why it stopped and whether this affects the predictions. This is discussed further in the section *Stopping Criteria*

If the calculation aborts it will conclude with a request to post the information on the web site's discussion board—please do—we can't fix it if we don't know it's broken.

Please post any problems on the discussion board on the code's discussion board.

10.2 Thermal stability and temperature convergence

This section describes thermal stability problems, how to identify them, and what to do about them.

10.2.1 Types of thermal maps

Three types of thermal maps, showing the heating or cooling of gas as a function of temperature, can be produced by CLOUDY. Each is the answer to a different question.

Figure 10.1 shows the heating and cooling rates as a function of temperature for a photoionized gas in which the gas kinetic temperature was varied. This figure was produced with the test case `func_map.in`, one of the standard test cases included in the code distribution. Both the gas density and the flux of ionizing photons were held constant and the kinetic temperature was varied. Only one temperature, the point where the two curves cross, occurs in equilibrium. The `func_map.in` file uses the **save map** command to determine heating and cooling rates at a variety of temperatures. This is exactly what the code does to determine the equilibrium temperature, so this plot can be useful to find out why the code ran into temperature convergence problems. This is why the command was introduced.

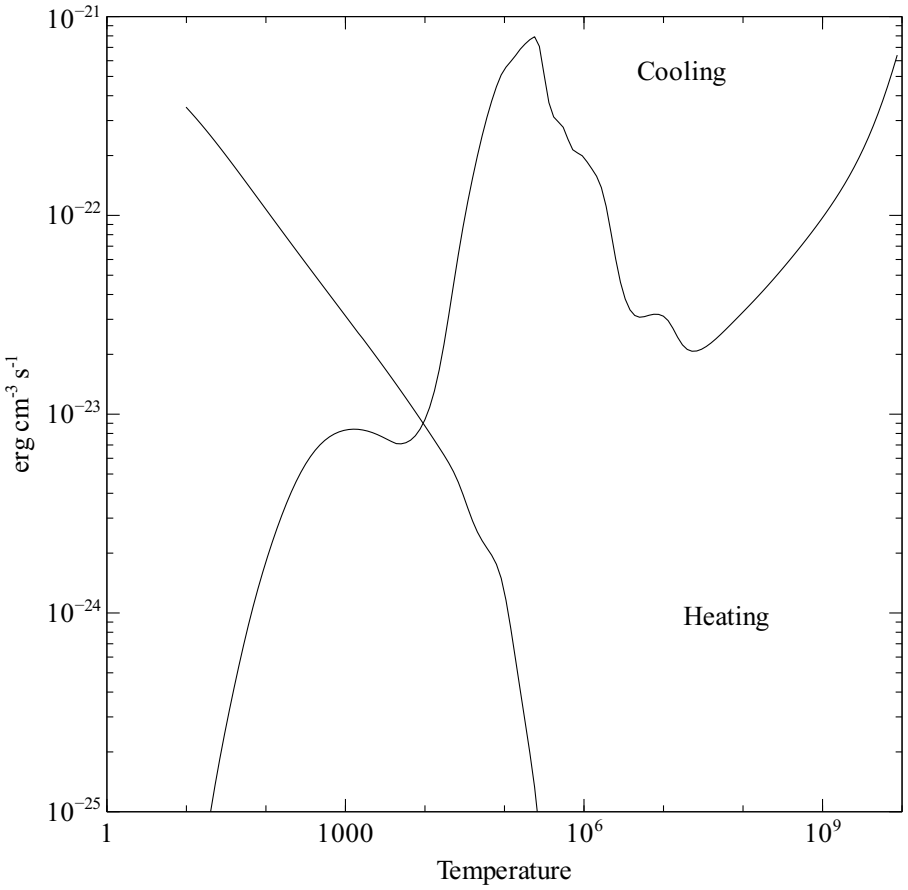

Figure 10.1: A typical heating—cooling function for low density photoionized gas. The cooling and heating rates (erg cm^{-3} s^{-1}) are shown.

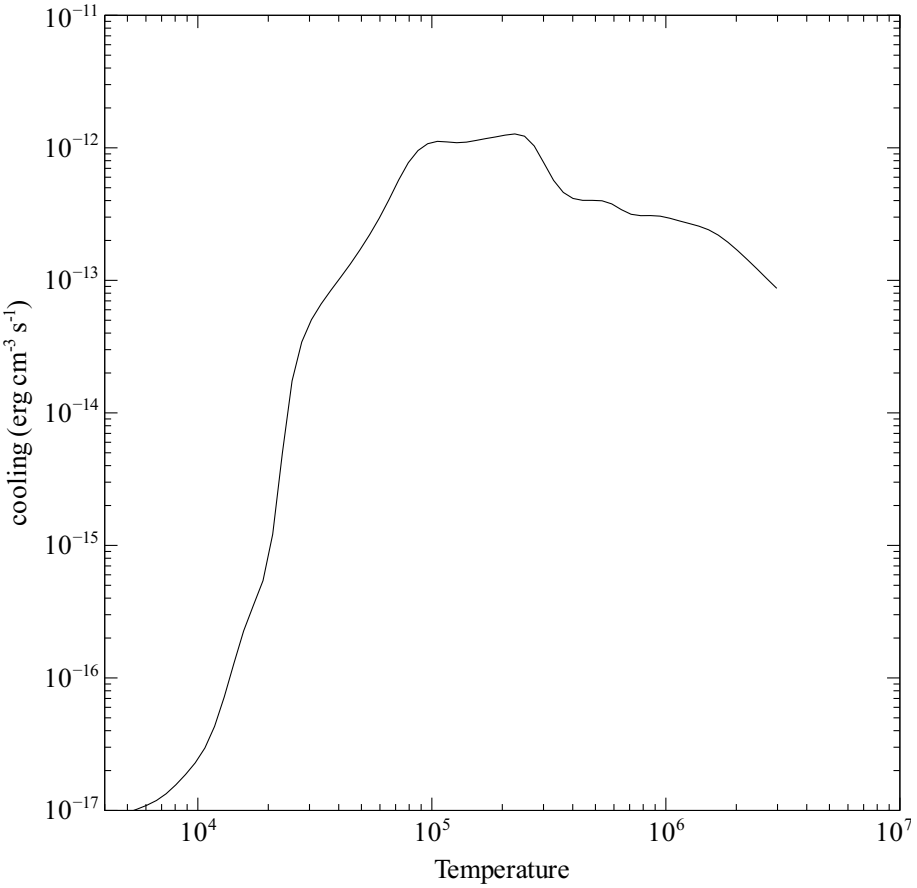

Figure 10.2: A typical cooling function for low density collisionally ionized gas.

Collisionally-ionized gas has a well-defined cooling rate that is only a function of temperature. The sample program `hazy_coolingcurve.cpp` (included in the `programs` directory in the code's distribution) does such a calculation, and Figure 10.2 shows the results. Here the kinetic temperature is set by some physics external to the calculation. The entire ionization solution is valid for each temperature under this assumption. The unspecified heat source would have to provide a local heating rate that is equal to the calculated cooling rate for the solution to be time steady.

The third map is the type of thermal stability map shown by Krolik et al. (1981) and plotted in Figure 10.3. The program that generated these results is given in the file `hazy_kmt.cpp`. Here the equilibrium temperature is determined self-consistently for gas over a wide range of densities, but for a single flux of ionizing photons (or equivalently, distance from the central object).

10.2.2 No Temperature Convergence

A temperature failure occurs when the heating-cooling balance is not within a certain tolerance, set by the **set temperature error** command, after 20 tries. Normally CLOUDY will punt after an excessive number of temperature failures occur. The limit to the number of failures is reset with the **failures** command. If the **failures map** command is entered then the code will first produce a

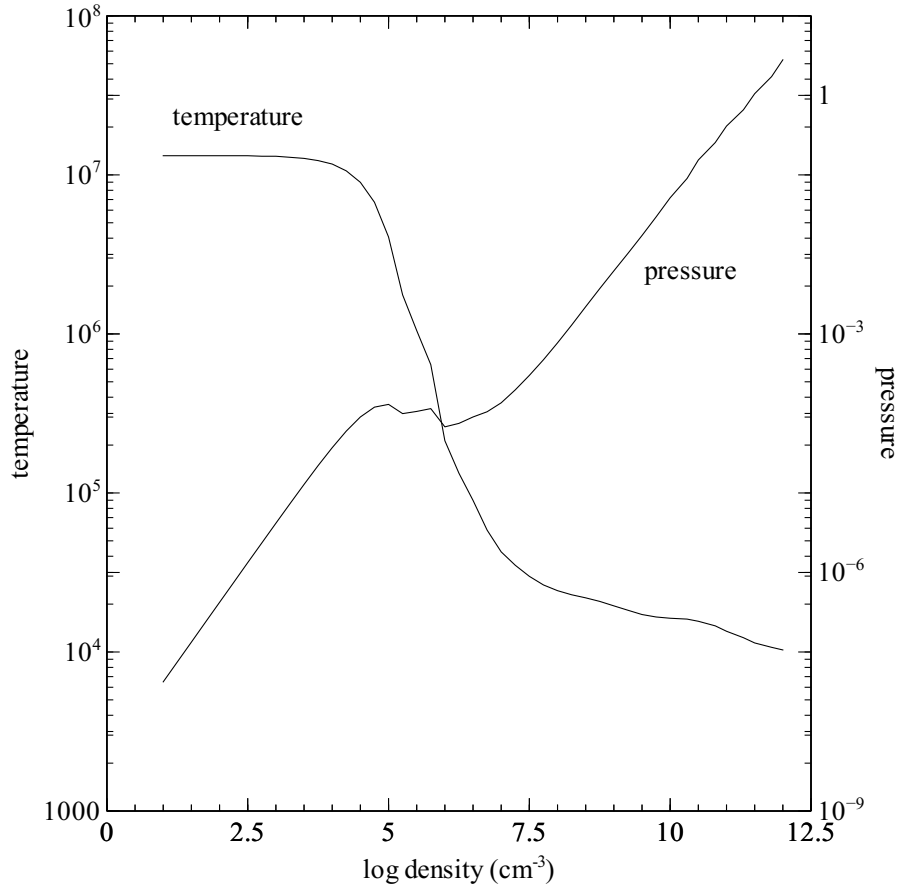

Figure 10.3: Equilibrium temperature as a function of density.

map of heating-cooling space to give an indication of where the equilibrium temperature should have been when excessive failures occur.

Temperature failures most often occur for temperatures in the range 10^2 K to 4×10^3 K, and 10^5 K to 10^6 K. These are where the cooling function permits more that one thermal solution (see, for example, Williams, 1967; Dalgarno and McCray, 1972).

Figure 10.1 shows a typical cooling function for gas in photoionization equilibrium. A peak is reached at a temperature near 10^3 K. This occurs when the fine-structure lines are major coolants. At lower temperatures their cooling rate increases exponentially (as expected), until roughly 10^3 K, when their Boltzmann factors are near unity. Above this temperature their cooling rate is nearly proportional to the Coulomb focusing factor $T^{-1/2}$, and the cooling *decreases* until the temperature is high enough for optical forbidden lines to become important (at roughly 4000 K). A similar phenomenon occurs near the $\sim 10^5$ K to 10^6 K peak in the cooling function.

When failures occur because more than one temperature solution is possible, the reported failures are a physical (not numerical) problem. CLOUDY will try to deal with this by forcing the temperature to values below the peak in the cooling function. Increasing the number of allowed failures (with the **failures** command) to prevent the code from stopping prematurely is permissible as long as the global energy balance is preserved. A warning will be issued at the end of the calculation if the heating-cooling balance is not preserved.

10.2.3 Thermal Stability

The thermal solution may be unstable when the temperature derivative of the net cooling function (cooling minus heating) is negative (Field, 1965). Possibly unstable solutions are indicated by a "u" just before the equilibrium temperature in the zone printout. The temperature derivative is for isochoric (constant density), not isobaric (constant pressure), conditions. Comments are printed at the end of the calculation if possibly unstable thermal solutions are present in the calculation.

10.2.4 Thermal fronts

Just as an ionization front is a region where the level of ionization changes dramatically over a small scale, a thermal front occurs where the temperature changes dramatically over a small scale. This can be caused by a real physical change of state of the gas such as those that occur near the peaks in the cooling curve. An example of a thermal front, taken from Ferland et al. (2002), is shown in Figure 10.4. This type of jump is physical. The gas changes phase and moves to different branches of the cooling curve. The code will generate a caution or comment if the electron temperature changes discontinuously from one zone to the next.

A thermal front can lead to pressure convergence failures when the solution jumps between the high and low temperature branches. Figure 10.5 shows an example case, taken from `orion_hii_pdr_pp.in` in the test suite. This shows the pressure history (output with the **save pressure history** command). The solver adjusts the density trying to make the resulting pressure agree with the desired pressure. The pressure changes continuously with density up to the point where the temperature jumps over the peak in the cooling curve. No solution is possible, and the code announces a pressure failure. In nature the presence of a magnetic field (added with the **magnetic field** command) will cushion the front from large changes in density.

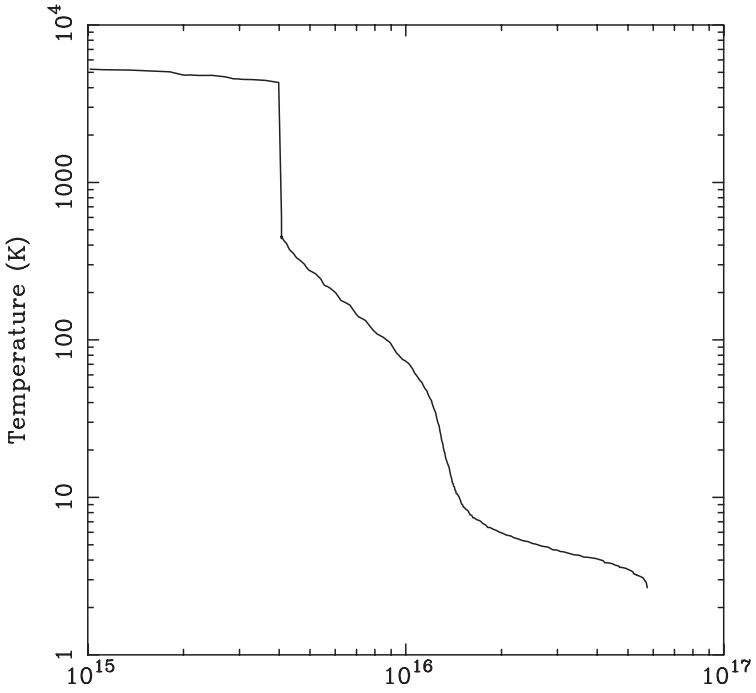

Figure 10.4: An example of a thermal front in a cooling flow cloud (Ferland et al., 2002). The x-axis is the depth into the cloud (cm). The thermal front at $\sim 4 \times 10^{15}$ cm is unresolved.

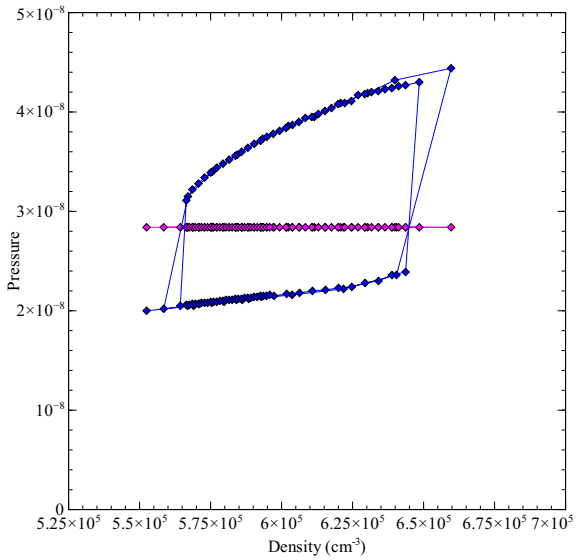

Figure 10.5: A thermal front in a constant pressure simulation. The x-axis gives the density [cm^{-3}] and the y-axis is the pressure [dynes cm^{-2}]. The points forming the large box are the resulting total gas pressure and the horizontal line is the correct pressure. The solution jumps above and below the equilibrium value as the temperature jumps above and below the thermal front.

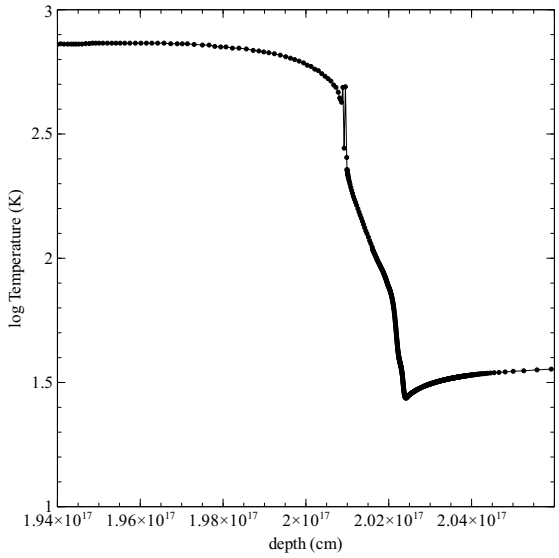

Figure 10.6: A constant-pressure thermal front in a temperature - radius plot. The x-axis gives the radius (cm). The y-axis gives the log of the temperature (K). The solution jumps above and below the equilibrium value, leading to a series of pressure failures, near a depth of 2×10^{17} cm, as it soldiers on through the thermal front.

A serious of pressure failures occur in this simulation when the gas falls to a temperature of ~ 300 K, as shown in Figure 10.6. The code simply presses on with the goal of reaching the cold side of the front.

10.2.5 Map Output

The program stops if an excessive number of temperature failures occur. The default limit is 20. It will produce a map of the heating and cooling as a function of temperature for the last computed zone if the **map** option on the **failures** command is given. The map is described here. The start of the output from the test case `func_map.in` is shown below.

```
90.02x map of heating vs cooling
 te, heating, cooling.
 Cloudy punts, Te= 9.254E+03 HTOT= 9.123E-24 CTOT= 9.118E-24 nzone=   1
 COOLNG array is
     O  4    25  0.340 O  3  5007  0.182 O  3    88  0.075 H FB     0  0.057 S  4    10
     H ff     0  0.022 S  3    33  0.020 Ne 3    15  0.019 Hefb     0  0.015 N  3    57
     Ne 5    24  0.010 Ne 5    14  0.009 C  3  1910  0.008 Heff     0  0.007 Si 2    34
 Line heating array follows
    Te     Heat------------------> Cool---------------------->    dH/dT    dC/DT
1.0000E+01 3.4774E-22   1   1 0.636 4.6095E-26 H FB    0A 0.723 -8.19E-24  1.56E-27 9.1
1.0209E+01 3.4490E-22   1   1 0.635 4.6814E-26 H FB    0A 0.720 -7.98E-24  1.65E-27 9.1
1.0423E+01 3.4233E-22   1   1 0.635 4.7510E-26 H FB    0A 0.717 -7.74E-24  1.74E-27 9.1
```

The output begins with a listing of the strongest coolants for the last zone. Then the program steps through increasing temperatures and prints the heating, cooling, and ionization of the gas.

From this information it should be possible to determine the temperature where the equilibrium thermal solution should have been. Each solution is completely self-consistent, except that heating and cooling do not balance. Both the local attenuated radiation field and collisional ionization contribute to the ionization balance at each temperature. All processes contribute to the thermal balance, including collisional ionization. The map is at constant density.

The first column gives the temperature. Columns 2 and 6 give the volume heating and cooling. Both have units erg s^{-1} cm^{-3}. Columns 3 and 4 constitute an indication of the main heating source. Columns 7 and 8 give the label and wavelength of the strongest coolant. Columns 5 and 9 give the fraction of the total heating or cooling due to these agents. Columns 10 and 11 give the heating and cooling derivatives. Columns 12 and 13 give the electron and hydrogen densities (cm^{-3}) and the remaining columns give the logs of the hydrogen and helium ionization fractions. The location of the probable thermal solution is indicated by a comment surrounded by dashed lines.

10.3 Convergence problems with dust-free static sphere

Ionization convergence problems can occur with a dust-free static spherical geometry. The default geometry when the **sphere** command is entered is for lines to freely escape after crossing the central hole due to some level of expansion. In a static spherical geometry (set with the **sphere static** command) the total Lα optical depth at the illuminated face of the shell will be very large since the line is scattered by the matter that lies across the entire shell. The line is destroyed when dust is present. If dust is not present the Lα intensity J will become very large. If the total optical depth in Lα is also large then the dominant escape / destruction process for the line will be absorption by atoms of third-row elements or the $n = 2$ level of hydrogen. This can lead to ionization convergence problems due to the extremely large Lα intensity J.

The first question to ask is whether this geometry is appropriate. Dust is nearly always present in the ISM. In dense stellar environments it is unlikely that a spherical geometry will be static. Include dust, use the default expanding spherical geometry, or a wind, and the problem will go away. To the best of my knowledge this geometry does not occur in nature.

10.4 Optical depth convergence problems

The code generally will not converge if it has not done so within ten or so iterations. Convergence problems most commonly occur when the specified column density or thickness is very near a prominent ionization front. In this case very small changes in the physical conditions result in large changes in the optical depths. The code will not have convergence problems if an optical depth is used as a stopping criterion instead.

10.5 Negative populations

It is possible that the code will stop because negative level populations were predicted for atoms, ions, or molecules. This is not supposed to occur, but sometimes happens because of numerical

instabilities in the matrix inversion routine. Please post the input stream and version of CLOUDY on the code's discussion board.

10.6 Floating Point Errors

The code should be compiled and linked with options enabled so that the code will crash on overflow or division by zero, but ignore underflow. The **crash** command described in Part 1 tests this. *Floating point errors should never occur.* The logic within the code is designed to identify problems, and complain, but not fail. The logic is only as good as the tests they were designed to pass. It is inevitable that circumstances will occur for which the logic now in the code is not sufficient. It is possible that the code will fail when these circumstances occur. I would be grateful for reports of any such failures, since they inevitably identify shortcomings in the code, and lead to its improvement. Please post comments on the discussion board on the code's web site.

10.7 We can't fix it if we don't know it's broken

Machines are growing faster far more rapidly than people are getting smarter. Reliability in the face of complexity is the major challenge to the development of any large-scale computer code (Ferland, 2001a). There can be little doubt that CLOUDY contains bugs.

If problems arise or the code crashes then it is likely that you found a problem. We would appreciate learning about such problems since they identify shortcomings which usually lead to improvements in the code (or the documentation). Please post queries and bug reports on the discussion board on the code's discussion board.

Chapter 11

HISTORY AND ACKNOWLEDGEMENTS

11.1 History

CLOUDY was born at the Institute of Astronomy, Cambridge, in August of 1978, in the computing environment described in the web document http://www.nublado.org/gary/computing1970s.htm. Its development has been continued at The University of Kentucky, The Ohio State University, and during extended visits to the Joint Institute for Laboratory Astrophysics, the Royal Greenwich Observatory, IOA Cambridge, Cerro Tololo Interamerican Observatory, and the Canadian Institute for Theoretical Astrophysics.

The code has been through three computer languages. It was originally written in FORTRAN IV and advanced through several dialects, reaching FORTRAN 77 in 1994 (version 84). Version 90 was written in a mix of FORTRAN 77 and MILSPEC extensions. This was the most advanced Fortran that could be used with open source compilers. It moved to ANSI 89 C in 1999 (version 96) and to C++ with the release of 07.02 in 2007.

Moore's Law is due to Gordon Moore, one of the founders of Intel Corporation. He observed that modern CPU's become about twice as powerful every 18 months. This trend has held true for the past twenty years, shows no sign of failing, and seems to be associated with our ability to control complexity. By this standard the growth of CLOUDY has been conservative, in that it is growing slower and complex on the Moore's-law timescale. Figure 11.1 shows the evolution of the code, as indicated by its size as a function of time.[1] As another example, the Meudon 1985 Meeting planetary nebula test (**pn_paris.in** in the test cases) has always taken about one minute to compute.

11.2 Acknowledgments

Comments or suggestions which led to the improvement of CLOUDY were made by the many individuals acknowledged on the web site http://www.nublado.org.

Peter G. Martin and Hagai Netzer had special roles during the early development of the code. Peter added several of the commands that deal with ordering of supplemental line lists and the

[1] Before mid-1995 the size was the total number of lines in the distributed source. After 1995 the size only includes the number of lines excluding block data. When the code was converted to C the block data were converted to external data files. These external files are now far larger than the code itself.

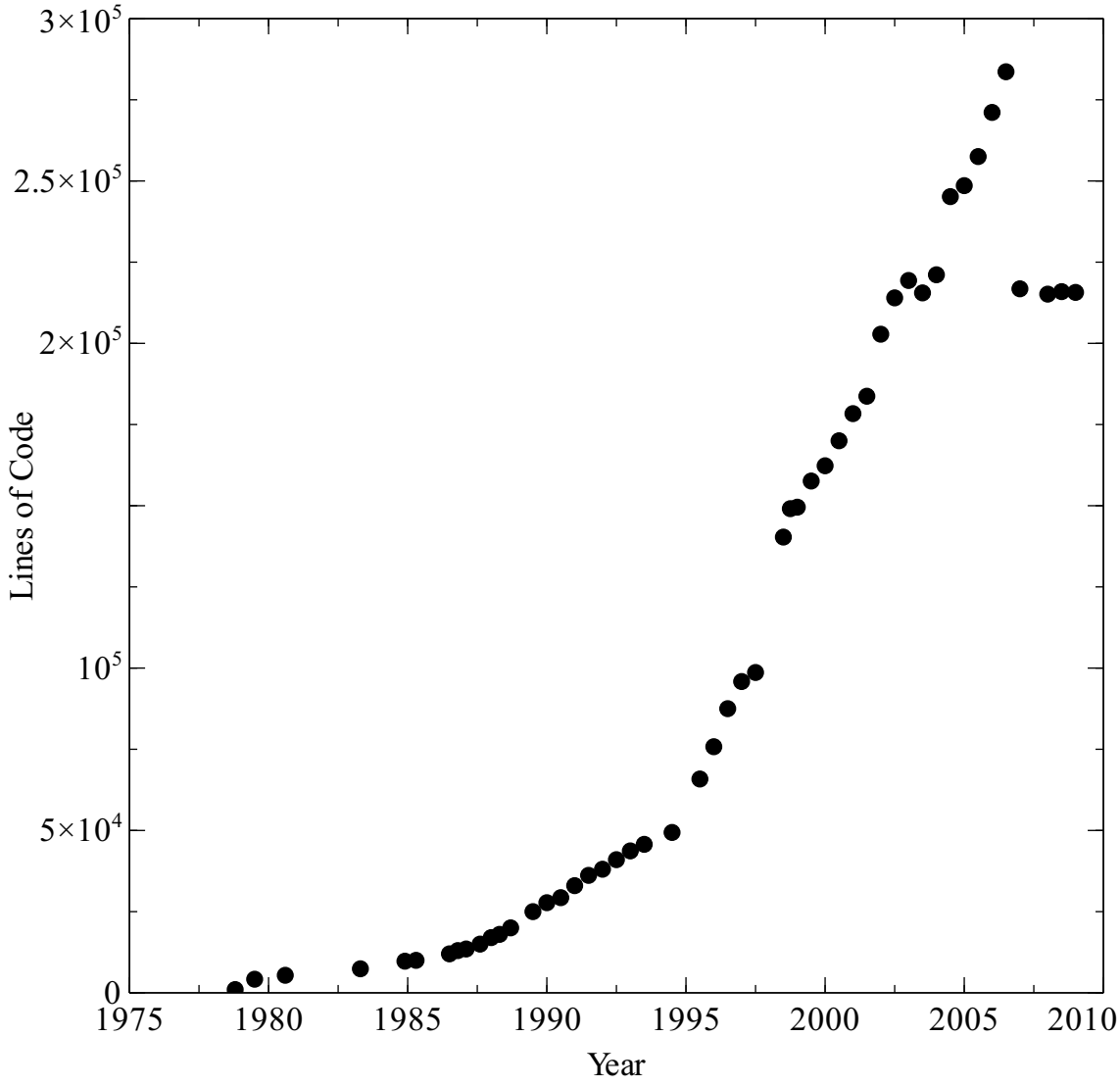

Figure 11.1: The size of the code as a function of time. The code grows roughly 7% larger per year, with growth spurts and slowdowns at times. There are several changes in slope evident - the year and cause are: 1985 - mainframe to Unix; 1993 - Unix to windows; the jump at 1999 - the Fortran to C conversion and the Williams / van Hoof drop in 2006, due to the use of object-like structures and moving converted fortran block data into separate files.

luminosity options on the **blackbody** command, insisted that CLOUDY run on a VAX, provided access to the University of Toronto VAX 11/780 during the 1980's, and more recently hosted the group at CITA during a sabbatical. Hagai and I have spent countless hours arguing over methods, assumptions, and just whose code had the bug. These comparisons are the only way to debug codes as large as CLOUDY or ION.

Peter van Hoof has gone over the code very carefully, finding many problems, and expanding its capabilities. The current version of the grain physics was developed by Peter together with Peter Martin, and Joe Weingartner. PvH developed the stellar library implementation in the current version. He is the maintainer for both the grains and stellar atmospheres codes.

The move to make the solvers far more rigorous and include dynamics and advection has been led by Robin Williams and Will Henney. Robin has rewritten the chemistry solvers to take advantage of the structures present in the C language and make them more robust.

The initial implementation of the hydrogen iso-electronic sequence was done by Jason Ferguson as part of his thesis. Ryan Porter developed the He-like isoelectronic sequence in his thesis. The expansion of the simulations into the PDR was done by Nick Abel and Gargi Shaw as part of their theses.

Sections of the code are taken from public domain software, as acknowledged in this document and in the source. Portions of the code were written by those listed in the `others.txt` file in the distributed files.

The preparation of the bibliographic references in this document made use of data from the NASA's Astrophysics Data System Bibliographic Services.

The development of CLOUDY 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 been continued with grants 83-05094, 85-12414, 87-19607, 90-19692, 93-19034, 96-17083, 00-71180, 03-0772, and most recently AST 06-07028. NASA has supported CLOUDY through ATP program awards NAG5-12020 and NNG05GD81G. Support from the University of Kentucky Center for Computational Sciences is also gratefully acknowledged.

Appendix A

ATOMIC DATA SOURCES

Codes like CLOUDY can only exist because of the large body of work done by the atomic and molecular physics community. This work will only continue to be supported if it is cited in the literature whenever it is used. The following is a partial list of citations for the atomic data used within the code.

This table is generated by the perl script `doc_atomic_data.pl`. This generates the file `doc_atomic_data_refer.txt` which is pasted below.

Appendix B

GLOSSARY OF SYMBOLS

As far as possible, the notation used by HAZY follows standard texts (AGN3; Mihalas, 1978). This is a summary of some of the symbols used.

The fundamental constants used by the code are from the CODATA recommended values. Constants are contained in the header `physconst.h`.

Symbol	Description	Units	Notes
a	Stefan radiation density	erg cm^{-3} K^{-4}	7.56464×10^{-15}
a	damping constant	—	
a_o	Bohr radius	$\hbar/m_e c^2$ cm	$0.5291775 \times 10^{-8}/Z$
A_{rad}	radiative acceleration	cm s^{-2}	
A_{ul}	radiative rate from level u to l	s^{-1}	
b_n	departure coefficient	—	
B	magnetic field	esu	
B_ν	Planck function	erg cm^{-2} s^{-1} Hz^{-1} sr^{-1}	
c	speed of light	cm s^{-1}	2.997925×10^{10}
C	collisional rate	s^{-1}	
C_{ul}	line collision rate	s^{-1}	
D_{ul}	line destruction probability	—	
f	oscillator strength	—	
$f(r)$	filling factor	—	
f_ν	flux density	erg cm^{-2} s^{-1} Hz^{-1}	
F_ν	flux density	erg s^{-1} Hz^{-1}	
g	grain asymmetry factor	—	
g_i	statistical weight	—	
g_{III}	T aver free-free gaunt factor	—	
$g_\odot$	Solar surface gravity	cm s^{-2}	2.74×10^4
G	gravitational constant	dyne cm^2 g^{-2}	6.673×10^{-8}
G	energy gains, heating	erg cm^{-3} s^{-1}	
h	Planck's constant	erg s	6.6262×10^{-27}
$\hbar$	Planck's constant	erg s	1.0546×10^{-27}
I	integrated intensity	erg s^{-1} sr^{-1} Hz^{-1}	
I_n	ionization potential of level n	erg Ryd	

I_ν	intensity	erg s^{-1} sr^{-1} Hz^{-1}	
J	integrated mean intensity	erg s^{-1} sr^{-1}	
J_ν	mean intensity	erg s^{-1} sr^{-1} Hz^{-1}	
k	Boltzmann constant	eV deg^{-1}	8.6171×10^{-5}
k	Boltzmann constant	erg deg^{-1}	1.38062×10^{-16}
$L_\odot$	luminosity of sun	erg s^{-1}	3.826×10^{33}
m_A	mass of atom A	gm	
$m_{\rm AMU}$	atomic mass unit	gm	$1.6605402 \times 10^{-24}$
m_e	electron mass	gm	9.10956×10^{-28}
m_e c^2	electron energy	Ryd	3.75584×10^{4}
m_p	proton mass	gm	$1.6726231 \times 10^{-24}$
M_J	Jeans' mass	gm	
$M_\odot$	mass of the sun	gm	1.989×10^{33}
$M_\oplus$	mass of the Earth	gm	5.977×10^{27}
n_e	electron density	cm^{-3}	
n_j	population of level j	cm^{-3}	
n_p	proton density	cm^{-3}	
$n(H)$	total H density, all forms	cm^{-3}	
$n(x)$	density of species x	cm^{-3}	
$n(cr)$	cosmic ray density	cm^{-3}	
n	atom's level	—	
$n(\mathrm{H}_{tot})$	H density, all forms	cm^{-3}	
N(x)	column density of species x	cm^{-2}	
$N(\mathrm{H}_{tot})$	total H col den, all forms	cm^{-2}	
$N_{\rm eff}$	effective H column density	cm^{-2}	
$P*$(x)	LTE relative population	cm^3	
P_{gas}	gas pressure	dyn cm^{-2}	
P_{lines}	line radiation pressure	dyn cm^{-2}	
P_{tot}	total pressure	dyn cm^{-2}	
P_{ul}	line escape probability	—	
$P_{\tau x}(n)$	continuum escape prob	—	
pc	parsec	cm	3.085678×10^{18}
q_{ij}	line collisional rate coefficient	cm^3 s^{-1}	
q_n	collisional rate coefficient	cm^3 s^{-1}	
q_e	electron charge	esu	4.80325×10^{-10}
$Q_{\rm abs}$	grain absorption efficiency	—	
Q(H)	hydrogen ionizing photons	s^{-1}	
r	radius	cm	
$r_{l,u}$	rate	s^{-1}	
R_0	inner radius	cm	
R	total to selective extinction	—	
$R_{\rm H}$	Rydberg unit for H	—	
R_∞	Rydberg unit for inf mass	—	
$R_{\rm AU}$	radius of Earth's orbit	cm	1.4959×10^{13}

R_+	radius of the Earth	cm	6.378×10^{18}
$R_\odot$	radius of the sun	cm	6.9599×10^{10}
T_e	electron temperature	cm^{-3}	
$T_{eff}(\odot)$	Sun's effective temperature	K	5770 K
T_{exc}	excitation temperature	K	
T_{color}	color temperature	K	
T_{low}	lowest temp allowed	K	2.8 K
T_u	energy density temperature	K	
u	energy density	$\mathrm{erg\ cm}^{-3}$	
U_g	grain potential	volt	
u	velocity (mean or projected)	$\mathrm{cm\ s}^{-1}$	
$\bar{u}$	mean particle speed	$\mathrm{cm\ s}^{-1}$	
u_{Dop}	Doppler velocity	$\mathrm{cm\ s}^{-1}$	
u_{exp}	expansion velocity	$\mathrm{cm\ s}^{-1}$	
u_{th}	thermal velocity	$\mathrm{cm\ s}^{-1}$	
u_{turb}	turbulent velocity	$\mathrm{cm\ s}^{-1}$	
V_g	grain potential	eV	
V_n	grain work function	eV	
W	geometric dilution factor	—	
x	relative shift from line center	—	
X_c	continuous to total opacity	—	
$\hat{Y}$	grain photoelectric yield	—	
year		s	3.156×10^7
z	redshift	—	
Z	nuclear charge	—	
α	Fine structure constant	$q_e^2/(\hbar c)$	1/137.036
$\alpha(n,T)$	recombination coefficient	$\mathrm{cm}^3\ \mathrm{s}^{-1}$	
$\bar{\alpha}(n,T)$	effec recomb coefficient	$\mathrm{cm}^3\ \mathrm{s}^{-1}$	
α_ν	continuous abs cross section	cm^2	
α_{lu}	line absorption cross section	cm^2	
α_β	Case B recomb rate coef	$\mathrm{cm}^3\ \mathrm{s}^{-1}$	
β	recombination cooling coef	$\mathrm{cm}^3\ \mathrm{s}^{-1}$	
η_ν	photon occupation number	—	
δr	zone thickness	cm	
Δr	depth into cloud	cm	
γ_u, l	continuum pumping probability	—	
Γ_n	photoionization rate	s^{-1}	
Γ	reciprocal lifetime of up level	s^{-1}	
Γ_{OTS}	OTS photoionization rate	s^{-1}	
κ	absorption opacity	cm^{-1}	
κ_{lu}	line absorption opacity	cm^{-1}	
κ_s	continuous scattering opacity	cm^{-1}	
κ_ν	continuous absorption opacity	cm^{-1}	
λ_J	Jeans' length	cm	

Λ	energy loss, cooling	erg cm^{-3} s^{-1}	
μ	mean molecular weight	—	
Ω	energy-specific collision strength	—	
Ω	shell coverage	sr	
$\Omega/4\pi$	covering factor	—	
Φ(H)	flux of ionizing photons	cm^{-2} s^{-1}	
$\phi\nu$	photon flux density	cm^{-2} s^{-1} Ryd^{-1}	
ϕ_{OTS}	flux of OTS photons	cm^{-2} s^{-1}	
ρ	mass density	gm cm^{-3}	
πa_o^2	area of first Bohr orbit	cm^2	87.9737×10^{-18}
	Classical electron radius	$q_e^2/(m_e c^2)$ cm	2.818×10^{-13}
σ_T	Thomson cross section	$8\pi/3 \times \left[q_e^2/(m_e c^2)\right]^2$ cm^2	6.6524×10^{-25}
σ_ν	scattering cross section	cm^2	
$\sigma_{\rm Ray}$	Rayleigh scat cross section	cm^2	
$\sum$	projected grain area	cm^2	
τ	optical depth	—	
τ_{abs}	absorption optical depth	—	
τ_{scat}	scattering optical depth	—	
$\tau_{u,l}$	line optical depth	—	
Υ	thermal averaged collision strength	—	
ν	frequency	Hz	
$\nu_{\rm Ryd}$	frequency	Ryd	
δ_ν	line width	Hz	
$\delta\nu_{\rm Dop}$	Doppler width	Hz	
χ_s	hν/kT	—	

Appendix C

CONVERSION FACTORS

Table C.1 gives conversion factors between various common units. The last column of the table gives the variable names for constants that occur within the code. Most are defined as macros within the header file **physconst.h**. These should be used instead of entering the constant directly. In the following all Rydbergs are for infinite mass nuclei.

The fundamental constants used by the code are from the CODATA recommended values and are in the header file `physconst.h`. Derived quantities should be formed from the fundamental quantities given there, so that any future changes will trickle down into all parts of the code.

Table C.1: Conversion Factors

To convert from	Variable	to	multiply by	Parameter
AU		cm	1.49597870(13)	
Boltzmann constant	BOLTZMANN	1.3806503(-16)		
cm		micron(μm)	10^4	
phot/s/cm^2	flux	f_ν	$\nu_{\rm Ryd} h\nu_1$ (erg)	
phot/Ryd/s/cm^2	flux/widflx	νf_ν	$\nu_{\rm Ryd}^2\ h\nu_1$ (erg)	
phot/Ryd/s/cm^2	flux/widflx	J_ν	$\nu_{\rm Ryd}$ h	
optical depth	tautot	A_V(mag)	1.08574	
energy (eV)		ergs	1.602192(−12)	
energy (eV)		K	1.1604448(4)	*eVdegK*
energy (keV)		Frequency Hz	2.41799(+17)	
energy (Ryd)	anu	Kelvin	1.5788866(5)	*Te1ryd*
energy (Ryd)	anu	ergs	2.179872(−11)	*en1ryd*
energy (Ryd)	anu	cm^{-1}	109737.315	*1/WavNRyd*
energy (Ryd)	anu	eV	13.6056981	*evRyd*
energy (Ryd)	anu	Å	911.6/energy(Ryd)	*rydlam*
energy (Ryd), T	anu, Te	hν/kT	1.5788866(5)*anu/Te	*Te1ryd*
temperature (K)	Te	eV	8.617385(−5)	
temperature (K)	Te	ergs	1.38063(−16)	*boltzmann*
temperature (K)	Te	Rydberg	1/1.5788866(5)	*1/te1ryd*
wavelength (Å)		meter	1(-10)	
wavelength (Å)		erg	1.9864(-8)/λ(Å)	
wavelength (Å)		degree K	1.43877(+8)/λ(Å)	
wavelength (cm)	micron	1(+4)		
wavelength (cm)	Å	1(+8)		
wavelength (cm)		ergs	1.9864(−12)/λ(cm)	
wavelength (cm)		degree K	1.43877/λ(cm)	
wavelength (cm)		Rydbergs	9.11256(−6)/λ(cm)	
wavelength (micron)		degree K	1.43877(+4)/$\lambda(\mu)$	
wavelength (micron)		ergs	1.9864(−12)/$\lambda(\mu)$	
wavenumbers (cm^{-1})		ergs	1.98648(−16)	
wavenumbers (cm^{-1})		degree K	1.43877	*WavNKelv*
wavenumbers (cm^{-1})		Rydberg	9.1126732(−6)	*WavNRyd*

Appendix D

THE TEST SUITES

D.1 Introduction

The code must be completely tested every time anything is changed. This is done with the test suite that is included in the distribution. The following pages list the test cases included in the `auto` directory within the test suite directory `tsuite`.

The test suite contains a series of Perl scripts that automate several tasks. The `readme_tests.htm` file included with the tests describes these scripts. The script `doc_tsuite.pl` extracts the test names and the description of each, and creates two files, `doc_tsuite.htm`, a formatted description of each test, and `doc_tsuite.txt`, the table that follows this discussion.

The test cases include a large number of **monitor** commands that allow the code to be automatically tested every night. These **monitor** commands have been removed from the examples below.

The simulations form various classes. The names of the classes and their intention is given in Table D.1.

D.2 Organization of commands

Commands can (mostly) occur in any order but we have made an effort to enter them in the order shown below. This is so that they can be studied to see examples of how to use the code.

 # commands controlling continuum

 # commands for density & abundances

 # commands controlling geometry

 # other commands for details

 # commands controlling output As indicated, there are the **print** and **save** commands which control the code's output.

 # commands giving the monitors Each test includes a number of **monitor** commands. These give values of predicted quantities that the code has obtained in the past. Changes to the code may cause predicted values to change, and if they do the **monitor** command will announce it.

Table D.1: Keywords used in the Test Suite.

Class	Function
Blr	Broad emission line region of AGN
Coronal	Collisionally ionized gas with pre-set temperature
Dynamics	Flow
Function	Test various functions of the code
Geometry	Test geometric aspects, aperture command
HII	H II regions
IGM	Intergalactic medium
ISM	Interstellar medium
Limit	Test limiting cases
NLR	Narrow-lined region of AGN
Nova	Aspects of the classical nova explosion
Optimizer	Test the optimizers
PDR	Photodissociation region
PN	Planetary nebulae
Stars	Stellar atmospheres

D.3 The Auto Test Suite

Table D.2 lists the simulations in the `auto` test directory.

Table D.2: The simulations in the auto test suite.

Class	Function
agn_blr_albedo	measure Rayleigh scattering of Lya
agn_lex00_u0	intermediate-ionization x-ray ionized cloud from Lexington 2000
agn_lex00_u1	high-ionization x-ray ionized cloud from Lexington 2000
agn_lex00_um1	low-ionization x-ray ionized cloud from Lexington 2000
agn_reflector	model of Compton reflector
agn_S_curve_grid	temperature across Spitzer thermal stability S curve
agn_warm_absorber	simple warm absorber model
agn_warm_absorber_hiU	simple warm absorber model
aperture_beam_int	test aperture beam command with intensity
aperture_beam_lum	test aperture beam command with luminosity
aperture_slit	test aperture slit command with luminosity
blr_f92	standard blr cloud in Ferland et al. 1992
blr_fp89	final F+P 1989 BLR model table 3
blr_hizqso	high Z quasar cloud
blr_kk81	old blr
blr_level2	test dominant level2 lines
blr_n09_p18	BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1
blr_n09_p18_Z20	BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

Continued on next page

Table D.2: (continued)

Class	Function
blr_n09_p20	BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
blr_n09_p20_Z20	BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
blr_n09_p22	BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
blr_n09_p22_Z20	BLR model, density 1e09 cm-3, flux of H-ion phots 1e22 cm2 s-1, Z=20
blr_n11_p20	BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1
blr_n11_p20_Z20	BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
blr_n12_p19	BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1
blr_n12_p19_Z20	BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1, Z=20
blr_n13_p18	BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
blr_n13_p18_Z20	BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
blr_n13_p22	BLR model, density 1e13 cm-3, flux of H-ion phots 1e22 cm2 s-1
blr_n13_p22_Z20	BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
blr_n14_p18	BLR model, density 1e14 cm-3, flux of H-ion phots 1e18 cm2 s-1
blr_n14_p20	BLR model, density 1e14 cm-3, flux of H-ion phots 1e20 cm2 s-1
blr_n14_p22	BLR model, density 1e14 cm-3, flux of H-ion phots 1e22 cm2 s-1
blr_nf84	early model of blr
blr_nf84_45deg	early model of BLR, with illumination at 45 degree angle
blr_rnfa	table 1 of Rees et al. ApJ 347, 648
blr_rnfb	table 1 of Rees et al. ApJ 347, 648
chianti_all_cool	cooling of a collisionally ionized plasma
chianti_fe_cool	cooling of a collisionally ionized plasma
coll_coronal	model of active region of solar corona
coll_heat_only	test code in limit where ONLY mechanical heating is present
coll_t3	coronal equilibrium at $10\hat{3}$ K
coll_t3_grains	coronal equilibrium at $10\hat{3}$ K, with grains to assist chemistry
coll_t4	coronal equilibrium at $10\hat{4}$ K
coll_t4_Z30	coronal equilibrium at $10\hat{4}$ K
coll_t5	coronal equilibrium at $10\hat{5}$ K
coll_t6	coronal equilibrium at $10\hat{6}$ K
coll_t7	coronal equilibrium at $10\hat{7}$ K
dynamics_orion_flow	Orion nebula blister with wind
dynamics_veryfast	very fast wind model
dynamics_veryfast_rec	very fast wind model
dynamics_wind	test of equations of motion in a very highly ionized wind
feii_hin	test feii in high density limit

Continued on next page

Table D.2: (continued)

Class	Function
feii_hirad	feii in case of high radiation density limit
feii_pump	test feii in continuum pumped limit
feii_ste	thermal equilibrium of FeII in STE limit
feii_t4n0	FeII emission in typical intermediate density photoionzied cloud
feii_t4n8	FeII emission in typical intermediate density photoionzied cloud
feii_t4n8_rt	FeII emission in typical intermediate density photoionzied cloud
feii_t4n8_Smyth19	FeII emission in typical intermediate density photoionzied cloud
feii_t4n8_Tayal18	FeII emission in typical intermediate density photoionzied cloud
feii_t4n8_Verner99	FeII emission in typical intermediate density photoionzied cloud
func_abund_fluc	check fluctuating heavy-element abundances
func_distance	check that distance and ”print flux earth” commands work
func_dlaw	test model with dlaw table
func_fulltrace	test full trace output
func_globule	test of globule command
func_grid_line_ratios	test generating line ratios in a grid run
func_grid_list	test the ’list’ keyword on the grid command
func_hotgas_coolstar	test very soft continuum, very hot gas
func_ion_increase	test model where ionization increases with depth
func_iso_large	test large iso sequence model atom
func_LineList_PDR	check that wavelengths agree at high line precision
func_LineList_PDR_H2	check that wavelengths agree at high line precision
func_LineList_PDR_H2_vacuum	check that wavelengths agree at high line precision
func_LineList_PDR_vacuum	check that wavelengths agree at high line precision
func_lines	create output file with list of func_lines
func_ly_pump_scale	test scaling of H lyman-line pumping
func_map	map of heating vs cooling
func_nolight	check OK with no radiation incident
func_sdrmin	test set drmin command
func_set_ion	test impact of setting ionization
func_stopcol	test stop column density ”species” command
func_stopline1	test stop line command
func_stopline2	test stop line command
func_t10	test very soft continuum, very hot gas
func_t3	test low temperature limit of code, 3K
func_t3_linesintroff	test low temperature limit of code, 3K
func_t3_linesoff	test low temperature limit of code, 3K
func_test	run smoke test
func_test_cycle	exercise full range of density, temperature
func_test_grid	test whether the output from a repeated model reproduces exactly
func_testmole	this runs the standard, one command, test, which contains many asserts

Continued on next page

Table D.2: (continued)

Class	Function
func_tlaw	test model with tlaw table
func_trans_lumi	test transmitted continuum in luminosity mode
func_trans_read	second of func_trans_save/func_trans_read pair, use transmitted continuum
func_trans_read_lumi_scale	test read transmitted continuum in luminosity mode
func_trans_read_scale	second of func_trans_save/func_trans_readread pair
func_trans_save	first of func_trans_save/func_trans_read pair, save continuum
func_trans_save_lumi	test save transmitted continuum in luminosity mode
grains_hot	test temperature of gas and dust in high energy density environment
grains_hot_wd01	test temperature of gas and dust in high energy density environment
grains_lte	check that grains equilibriate at correct temp in ste limit
grains_qheat	cool atomic ISM with Si grain quantum heating
grains_temp	test all grain species temperature
grains_temp_all	test all grain species temperature
grd_extreme_THiNhi	slow/grid_extreme highest density highest temperature
grd_extreme_ThiNlo	slow/grid_extreme lowest density highest temperature
grd_extreme_TloNhi	slow/grid_extreme highest density lowest temperature
grd_extreme_TloNlo	slow/grid_extreme lowest density lowest temperature
grid_coronal	coronal equilibrium
grid_coronal_grains	coronal equilibrium
grid_coronal_primal	coronal equilibrium
grid_h2coronal	coronal equilibrium
grid_h2coronal_primal	coronal equilibrium
h2_coll_t4	coronal equilibrium at 10$\hat{4}$ K
h2_cr	H2 with background cosmic ray ionization
h2_cr_grains	background cosmic ray ionization by suprathermal electrons only
h2_hminus	H2 populations in H- dominated limit
h2_pdr_leiden_f1	low density and flux model 1
h2_solomon	H2 populations in solomon dominated limit
h2_t2000	test large H2 molecule in shock-like conditions
h2_t500	test large H2 molecule in PDR-like conditions
h_otsopen	test ots, inward fractions for pure hydrogen, open geo, filling factor
h_otspp	plane parallel conservation and hydrogenic emission for pure hydrogen
h_otssp	spherical conservation and hydrogenic emission for pure hydrogen
h_outopen	test open geometry
h_outpp	plane parallel H-only, close, test hydrogenic emission
h_outsp	spherical conservation and hydrogenic emission for pure hydrogen
h_t4_conemis	continuous emission from H atom
h_t4_conemis_lon	low-den continuous HI emission with 2-nu important
h_t4_conemis_thick	H I continuous emissivity, used for plot in hazy

Continued on next page

Table D.2: (continued)

Class	Function
heatomt10	continuous emission from HeI
heatomt10lon	test low-den continuous emission from H atom, 2-nu is important
heiont10	continuous emission from HeII
helike_ar	He-like argon emission
helike_c	he-like carbon emission
helike_co	He-like cobalt emission
helike_cu	He-like copper emission
helike_fe	he-like iron emission
helike_mg	he-like magnesium emission
helike_n	He-like nitrogen emission
helike_ne	he-like neon emission
helike_ni	he-like nickel emission
helike_o	he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
helike_si	He-like silicon emission
helike_zn	He-like zinc emission
hhe_otspp	plane parallel conservation and H-like emission for H, He
hhe_otssp	spherical conservation and H-like emission for H and He
hhe_outpp	plane parallel conservation emission for H, He gas
hhe_outppff	plane parallel filling factor pure H, He gas
hhe_outsp	spherical conservation and H-like emission for H, He
hii_blister	Lexington 1995 dust-free hii blister region
hii_coolstar	dust free cool HII region model, Lexington 1995
hii_hiU_StaticSphere_noGrains	very high ionization parameter static H II region without dust
hii_hiU_StaticSphere_noGrains	test
hii_icf	HII region with negative He/H ICF
hii_paris	”New” Paris meeting HII region
hii_Um3	H II region sim from Christophe Morriset’s ionization paramter family
hii_Um35	H II region sim from Christophe Morriset’s ionization paramter family
hii_Um385	H II region sim from Christophe Morriset’s ionization paramter family
hlike_c	H-like C VI case B
hlike_o	H-like O VIII case B
igm_lalpha	Ly alpha forest cloud
igm_lalpha_hm12	Ly alpha forest cloud
igm_lalpha_noisosub	Ly alpha forest cloud
igm_lalpha_noisosub_hm12	Ly alpha forest cloud
igm_perseus	Perseus cluster
igm_primal	cloud with primordial abundances exposed to background at Z=10
igm_z3	redshift 1000 recombination epoch

Continued on next page

Table D.2: (continued)

Class	Function
igm_z3_thick	redshift 1000 recombination epoch
ism	cloud irradiated by ism background
ism_cosmicray	background cosmic ray ionization by suprathermal electrons only
ism_grid	interstellar cloud irradiated by ism background
ism_hot_brems	generate continuum due to hot ism in high Z,z starburst
ism_jura	check rate H2 forms on grain surfaces
ism_opacity	generate standard ISM opacity curve
ism_set_cr_rate	background cosmic ray ionization by suprathermal electrons only
limit_casea_h_den13	case A
limit_casea_h_den_temp	Test model H in Case A limit
limit_caseb_h_den10_temp45	the best we can do to predict the H I emission spectrum
limit_caseb_h_den2_temp37	the best we can do to predict the H I emission spectrum
limit_caseb_h_den2_temp4	the best we can do to predict the H I emission spectrum
limit_caseb_h_den2_temp45	the best we can do to predict the H I emission spectrum
limit_caseb_h_den2_temp5	the best we can do to predict the H I emission spectrum
limit_caseb_h_den2_temp5_coronal	the best we can do to predict the H I emission spectrum
limit_caseb_h_den4_temp45	the best we can do to predict the H I emission spectrum
limit_caseb_h_hs87	”Case B from Hummer and Storey”
limit_caseb_h_lot	log density case B, T=500 log n=2
limit_caseb_h_n8	h_caseb_n8 high density case B
limit_caseb_he2_den8	limit_caseb_he2_den8 He II case B
limit_caseb_he_den	Test model H and He atoms in Case B limit
limit_caseb_he_den2_temp4	the best we can do to predict the HeI emission spectrum
limit_caseb_he_den4_temp4	the best we can do to predict the HeI emission spectrum
limit_caseb_he_den4_temp4_Fuji	the best we can do to predict the HeI emission spectrum
limit_caseb_he_den4_temp4_VR62	the best we can do to predict the HeI emission spectrum
limit_caseb_he_den4_temp4_VS80	the best we can do to predict the HeI emission spectrum
limit_caseb_he_den_temp	Test model He atoms in Case B limit
limit_caseb_hhe_den	Test model H and He atoms in Case B limit
limit_caseb_hhe_den_temp	Test model H and He atoms in Case B limit
limit_casec_h_den2	H only optically thin in Lyman continuum
limit_casec_h_den5	case C
limit_compton_hi_t	test high-T Compton energy exchange
limit_compton_lo_t	test low-T Compton energy exchange
limit_compton_mid_t	mid-T Compton energy exchange
limit_conserve	test that energy is limit_conserved
limit_eden	Martin Gaskell’s funny model
limit_h_induc	constant temper black body limit from Ferland and Rees 1988
limit_hi_ion	very high ionization parameter limit
limit_laser_1	test of H ionization in optically thin limit
limit_laser_2	test of H and HeI ionization in optically thin limit

Continued on next page

Table D.2: (continued)

Class	Function
limit_laser_200	ionization in Auger-dominated limit
limit_laser_200_low	test ionization in Auger-dominated limit
limit_laser_3	test H and He ionization in optically thin limit
limit_lowd0	test low density limit
limit_lowden	test optically thin model that extends to very low densities
limit_lowdm6	test low density limit
limit_lowion	test conditions of very low ionization matrix solver
limit_lte_h_t50_cion	collisionally ionized H in LTE limit
limit_lte_h_t50_coll	collisionally excited H in LTE limit
limit_lte_he1_coll	He atom at high densities
limit_lte_he1_nomole_iso_force	He atom in LTE at high densities, with no molecules, iso forced to LTE
limit_lte_he1_nomole_ste	He atom in LTE at high densities, with no molecules
limit_lte_he1_nomole_ste_nocoll	He atom in LTE at high densities, with no molecules and no collapsed levels
limit_lte_he1_nomole_ste_nocoll2	He atom in LTE for a large range of Te and density, with no molecules and no collapsed levels and no collisions
limit_lte_he1_ste	He atom in LTE at high densities
limit_lte_hhe_coll_t50	H, He in LTE at high densities
limit_lte_hhe_induc	radiation dominated H, He gas goes to STE
limit_lte_hhe_ste	H, He in STE
limit_lte_hminus	H- goes to LTE
limit_lte_metal	STE with metals
limit_recoil_ion	test compton recoil ionization of hydrogen
limit_strom	pure-H Stromgren sphere
limit_supra	secondary ionization dominated gas
limit_thick_brems	optically thick brems
limit_vbhum	compare with Van Blerkom and Hummer exact RT results
limit_veryveryfast	very fast simulation for Purify/valgrind
lya-21cm-constant	test effect of lya pump on spin temperature
lya-21cm-excitation	test effect of lya pump on spin temperature
lya-21cm-kinetic	test effect of lya pump on spin temperature
nlr_lex00	NLR model for Lexington 2000 Meeting
nlr_liner	NLR liner model
nlr_liner_grains	liner model with grains
nlr_paris	Paris meeting NLR model
nova_dqher	cold nova shell
nova_photos	dense nova photosphere
optimize_phymir	test phymir optimizers
optimize_subplex	test subplex optimizer
orion_hii_open	conditions similar to Orion nebula blister

Continued on next page

Table D.2: (continued)

Class	Function
orion_hii_pdr	constant pressure H+ region/pdr
orion_hii_pdr_fast	constant gas pressure H+ region/PDR
pdr_co_fully	H2 and CO in fully molecular limit
pdr_co_fully_noneq	H2 and CO are fully molecular, non-equilibrium case
pdr_coolbb	illumination by cool STE blackbody
pdr_dense_persei	dense phase zeta persei cloud
pdr_HTT91	low-density PDR from HTT91
pdr_leiden_f1	Leiden meeting model 1
pdr_leiden_f2	Leiden meeting model 2
pdr_leiden_f3	Leiden meeting model 3
pdr_leiden_f4	Leiden meeting model 4
pdr_leiden_hack_f1	Leiden meeting model 1 with hacks
pdr_leiden_hack_f2	Leiden meeting model 2 with hacks
pdr_leiden_hack_f3	Leiden meeting model 3 with hacks
pdr_leiden_hack_f4	Leiden meeting model 4 with hacks
pdr_leiden_hack_v1	Leiden meeting model 5 with hacks
pdr_leiden_hack_v2	Leiden meeting model 6 with hacks
pdr_leiden_hack_v3	Leiden meeting model 7 with hacks
pdr_leiden_hack_v4	Leiden meeting model 8 with hacks
pdr_leiden_v1	Leiden meeting model 5
pdr_leiden_v2	Leiden meeting model 6
pdr_leiden_v3	Leiden meeting model 7
pdr_leiden_v4	Leiden meeting model 8
pdr_minimal	test physical conditions at the illuminated face of a PDR
pdr_orion_veil	Orion's veil
pdr_th85ism	TH85 PDR with ISM grains
pdr_th85ism_cgto	TH85 pdr with ISM grains and C ¿ O
pdr_th85orion	TH85 PDR with Orion grains
pn_fluc	Paris PN with density fluctuations
pn_ots	Paris PN with ots
pn_paris	"Paris meeting PN"
pn_paris_cpre	"Paris meeting PN with constant pressure"
pn_paris_fast	Paris PN, fast version
pn_sqrden	PN with density propt R^2 and filling factor
rrc_o	he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
stars_atlas	Atlas stellar atmosphere
stars_atlas_3d	Atlas stellar atmosphere, 3D interpolation
stars_atlas_all	interpolate on Atlas grids
stars_atlas_odfnew_all	access various Atlas ODFNEW grids
stars_bstar2006	tlusty bstar grid
stars_bstar2006_3d	tlusty bstar grid

Continued on next page

Table D.2: (continued)

Class	Function
stars_bstar2006_all	tlusty bstar grid
stars_costar1	costar interpolation mode 1
stars_costar2	costar interpolation mode 2
stars_costar3	costar interpolation mode 3
stars_costar4	costar interpolation mode 4
stars_costarhalo	costar halo abundances
stars_kurucz79	Kurucz 1979 SED
stars_mihalas	Mihalas SED
stars_obstar_merged	tlusty bstar grid
stars_obstar_merged_3d	tlusty bstar grid
stars_obstar_merged_all	tlusty bstar grid
stars_optimize1	optimizer on stellar grids
stars_optimize2	optimizer on stellar grids
stars_optimize3	optimizer on stellar grids
stars_ostar2002	tlusty O star grid
stars_ostar2002_3d	tlusty Ostar grid
stars_ostar2002_all	tlusty Ostar grid
stars_rauch_3d	Rauch 3-dimensional grid
stars_rauch_cowd	Rauch hot PN star
stars_rauch_h+he	Rauch PN central star
stars_rauch_h-ca	Rauch central star hot PN
stars_rauch_h-ni	Rauch hot PN star
stars_rauch_helium	Rauch hot PN star
stars_rauch_hydr	Rauch hot PN star
stars_rauch_pg1159	Rauch hot [WR] PN
stars_rauch_pg1159_ascii	Rauch cool [WR] PN
stars_starburst99	Starburst 99 SED
stars_starburst99_2d	Starburst 99 2D SED
stars_werner	Werner stars grid
stars_wmbasic	wmbasic stellar SED
thin	”Thin coronal model”
time_cool_cd	constant density cooling cloud
time_cool_cd_eq	constant density equilibrium cooling cloud
time_cool_cd_flux	constant density cooling cloud
time_cool_cd_noaccu	constant density cooling cloud

This HTML file was created by the program doc_tsuite.pl, doc_tsuite.txt contains a tab delimited list of the files.

---

agn_blr_albedo.in

measure Rayleigh scattering of Lya

```
title measure Rayleigh scattering of Lya
# model from Korista, K., & Ferland, G. 1998, ApJ, 495, 672
#
# commands controlling continuum =========
agn 6.683 -1.20 -1.20 -0.90
ionization parameter 1.0
#
# commands for density & abundances =========
init file = "ism.ini"
abundances old solar 84
hden 11.0
#
# commands controlling geometry =========
stop total column density = 23.75
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "C 6" 33.7360
print line faint -1
print lines inward
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "agn_blr_albedo.ovr"
save performance "agn_blr_albedo.per"
save continuum last "agn_blr_albedo.con" units kev
save dr "agn_blr_albedo.dr"
save reflected continuum last "agn_blr_albedo.ref"
save emitted continuum last "agn_blr_albedo.emt"
#
# must assert the luminosity since change in this
# line would appear to change the rest of the spectrum
# agn_blr_albedo.in
# class blr
# ========================================
```

This model computes the albedo of a fairly standard BLR cloud. This is the type of model that was presented in the BLR albedo paper by Korista & Ferland, 1998, ApJ 495, 672.

The asserts then check that these continua have the expected brightness.

---

agn_lex00_u0.in

intermediate-ionization x-ray ionized cloud from Lexington 2000

```
title intermediate-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print line sort wavelength
print lines column linear
normalize to "H 1" 1215.67A
print line faint -1
hden 5
iterate
```

```
phi(h) 15.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
#
save overview "agn_lex00_u0.ovr"
save performance "agn_lex00_u0.per"
save transmitted continuum "agn_lex00_u0.trn" units keV
#
# agn_lex00_u0.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

---

agn_lex00_u1.in

high-ionization x-ray ionized cloud from Lexington 2000

```
title high-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print lines column linear
normalize to "H 1" 1215.67A
print line faint -1
hden 5
iterate
phi(h) 16.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
```

```
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
save overview "agn_lex00_u1.ovr"
save performance "agn_lex00_u1.per"
save transmitted continuum "agn_lex00_u1.trn" units keV
#
# agn_lex00_u1.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

---

agn_lex00_um1.in

low-ionization x-ray ionized cloud from Lexington 2000

```
title low-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print lines column linear
print lines sort intensity
normalize to "H 1" 1215.67A
print line faint -2
hden 5
iterate
phi(h) 14.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
```

```
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
#
save overview "agn_lex00_um1.ovr"
save performance "agn_lex00_um1.per"
save transmitted continuum "agn_lex00_um1.trn" units keV
#
# agn_lex00_um1.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

`agn_reflector.in`

model of Compton reflector

```
title model of Compton reflector
#
# commands controlling continuum =========
# this is a powerlaw that extends into the x-rays, but by default
# has exponential cutoff in FIR
power law -1. hi=1000000000
# the ionization parameter for this powerlaw
ionization parameter 1.
# add background so that FIR/radio does not have zero flux
background
iterate
#
# commands for density & abundances =========
hden 11
#
# commands controlling geometry =========
stop total column density 24
#
# other commands for details =========
constant temper 5
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 10
```

```
#
# commands controlling output =========
print line faint 1
print line inward
#
# this is to produce lines with lots of contrast with the continuum
set save Line Width 100 km/sec
# a fig in part 3 of hazy uses data from this model. the fig shows lines
# with above and below linewidth
# set save line Width c
save performance "agn_reflector.per"
save continuum last "agn_reflector.con" units kev
save continuum reflected last "agn_reflector.alb" units kev
save overview last "agn_reflector.ovr"
save dr last "agn_reflector.dr"
#
# agn_reflector.in
# class blr
# ======================================
#
```

This is a model of the Compton reflector in AGN. It is a constant temperature since models of this region often make that assumption. A plot in Part I of Hazy shows the incident and reflected portions of the continuum. The code will complain that the cloud is Compton thick since it is not really designed to simulate this situation.

`agn_S_curve_grid.in`

temperature across Spitzer thermal stability S curve

```
title temperature across Spitzer thermal stability S curve
#
# commands controlling continuum =========
# this is the generic AGN continuum
table agn
# the ionization parameter will be varied
ionization parameter 0.00 vary
grid from 0 to 3 in 0.25 dex steps sequential
# add background so that FIR/radio does not have zero flux
background
iterate
#
# commands for density & abundances =========
# intended to make sim run as fast as possible
hden 8
init file "ism.ini"
element sulphur off
element chlorine off
element argon off
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output
# this produces a very large number of lines in the output mostly
# because Hbeta is very weak in hot gas. Choose Lya as the normalization
# line to make line list smaller
normalize to "H 1" 1215.67A
print line faint 10 will be varied
# create file with list of grid parameters
save overview "agn_S_curve_grid.ovr" last no hash
save performance "agn_S_curve_grid.per"
save grid "agn_S_curve_grid.grd" last no hash
save species densities "agn_S_curve_grid.sden" "Si+12[10:11]" last no hash
# save average H+ temperature
```

```
save average "agn_S_curve_grid.avr" last no hash
temperature hydrogen 1
end of temperatures
# save heating and cooling
save heating "agn_S_curve_grid.het" last no hash
save cooling "agn_S_curve_grid.col" last no hash
save pressure "agn_S_curve_grid.pre" last no hash
save iron element "agn_S_curve_grid.fe" last no hash
save xspec atable "agn_S_curve_grid.fit"
save neon element "agn_S_curve_grid.ne" last separate
#
#
# agn_S_grid.in
# class BLR
# ======================================
#
```

This computes a series of models that check the temperature through the S curve in the Fields et al. three-phase model of ISM stability.

`agn_warm_absorber.in`

simple warm absorber model

```
title simple warm absorber model
#
# commands controlling continuum =========
table power law
ionization parameter 0
#
# commands for density & abundances =========
hden 6
abundances old solar 84
#
# commands controlling geometry =========
stop column density 22
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint 10
save overview "agn_warm_absorber.ovr"
save performance "agn_warm_absorber.per"
save continuum "agn_warm_absorber.con" last units kev
save continuum "agn_warm_absorber.conA" last units Angstroms
save fine continuum "agn_warm_absorber.finA" last units Angstroms range 7.6A to 15A merge 3
save dr "agn_warm_absorber.dr" last
save lines, optical depth some, "agn_warm_absorber.opt" last
O 3 5006.84A
end of lines
# this will be the default units, like the printout
save line optical depths last "agn_warm_absorber_lab.lin"
# this will be the same, in rygbergs
save line optical depths last "agn_warm_absorber_ryg.lin" units rydberg
#
# warrm_absorber
# class nlr
# ======================================
#
```

this is a simple warm absorber model. It makes a plot of the transmitted continuum, and generates a list of lines with significant optical depths

---

agn_warm_absorber_hiU.in

simple warm absorber model

```
title simple warm absorber model
set save prefix "agn_warm_absorber_hiU"
#
# commands controlling continuum =========
table power law
ionization parameter 150 linear
#
# commands for density & abundances =========
hden 6
abundances old solar 84
#
# commands controlling geometry =========
stop column density 22
#
# commands controlling models =========
database h-like element zinc collapsed levels 5
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line column
normalize "Blnd" 1.77982A
save overview ".ovr"
save performance ".per"
save continuum ".con" last units kev
save continuum ".conA" last units Angstroms
save fine continuum ".finA" last units Angstroms range 7.6A to 15A merge 3
save dr ".dr" last
# this will be the default units, like the printout
save line optical depths last ".linkev" unit kev
# this will be the same, in angstrom
save line optical depths last ".lina" -3 units angstrom
#
# warrm_absorber
# class nlr
# ======================================
#
```

This is simple warm absorber model with a high ionization parameter, chosen to yield about 50% ionization fractions for H-like Fe and Zn. It generates a list of lines with significant optical depths.

---

aperture_beam_int.in

test aperture beam command with intensity

```
title test aperture beam command with intensity
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# other commands for details =========
constant temper 4
#
# commands controlling continuum =========
laser 2
ionization -2
```

```
#
# commands controlling geometry =========
stop thickness 10
sphere
aperture beam
#
# commands controlling output =========
save overview "aperture_beam_int.ovr"
save performance "aperture_beam_int.per"
#
# aperture_beam_int.in
# class geometry
# ======================================
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a beam contered on the center of the nebula, with a line of sight extending through the object.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that the emission line has the correct "luminosity". In this case the inner radius is not specified so the returned value is unity.

`aperture_beam_lum.in`

test aperture beam command with luminosity

```
title test aperture beam command with luminosity
#
# commands controlling continuum =========
laser 2
q(h) 31.5
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# commands controlling geometry =========
stop thickness 1e10 linear cm
radius 9
sphere
aperture beam
#
# other commands for details =========
constant temper 4
#
# commands controlling output =========
save overview "aperture_beam_lum.ovr"
save performance "aperture_beam_lum.per"
#
# aperture_beam_lum.in
# class geometry
# ======================================
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a beam contered on the center of the nebula, with a line of sight extending through the object.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that this emission line has the correct "luminosity".

aperture_slit.in

test aperture slit command with luminosity

```
title test aperture slit command with luminosity
#
# commands controlling continuum =========
laser 2
q(h) 31.5
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# commands controlling geometry =========
radius 9 10
sphere
aperture slit
#
# other commands for details =========
constant temper 4
#
# commands controlling output =========
save overview "aperture_slit.ovr"
save performance "aperture_slit.per"
#
# aperture_slit.in
# class geometry
# ======================================
#
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a long slit contered on the center of the nebula, extending beyond the outer reaches of the matter.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that the emission line has the correct "luminosity".

---

blr_f92.in

standard blr cloud in Ferland et al. 1992

```
title standard blr cloud in Ferland et al. 1992
#
# commands controlling continuum =========
table agn
ionization parameter -1
#
# commands for density & abundances =========
hden 11
abundances old solar 84
#
# commands controlling geometry =========
stop column density 25
#
# other commands for details =========
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 10
```

```
iterate to convergence
#
# commands controlling output =========
print h-like departure hydrogen
print h-like populations hydrogen
print h-like departure helium
print h-like populations helium
normalize to "H 1" 1215.67A = 105.90
print line faint -2
save performance "blr_f92.per"
save overview last "blr_f92.ovr"
save convergence reason "blr_f92.cvr"
save element nitrogen last "blr_f92.nit"
save element calcium last "blr_f92.ca"
save dr "blr_f92.dr"
save transmitted continuum "blr_f92.trn" last
#
# blr_f92.ini
# class blr
# ======================================
```

This is similar to one of the BLR models presented in Ferland et al. (1992) for the well-studied Seyfert galaxy NGC 5548. It has a very large column density and is marginally optically thick to electron scattering. The spectrum is given relative to Lya, and the intensity of this line is reset to produce a spectrum that is on the same intensity scale as that paper.

`blr_fp89.in`

final F+P 1989 BLR model table 3

```
title final F+P 1989 BLR model table 3
#
# commands controlling continuum =========
table agn
ionization parameter -0.5
#
# commands for density & abundances =========
hden 9.5
init file="c84.ini"
abundances old solar 84
#
# commands controlling geometry =========
stop column density 25.5
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
# set a relatively high faint level since lines relative to Lya=100
print line faint -1
print h-like departure coefficients hydrogen
normalize to "H 1" 1215.67A = 85.60
save performance "blr_fp89.per"
save heating "blr_fp89.het"
save convergence reason "blr_fp89.cvr"
save cooling "blr_fp89.col"
save overview last "blr_fp89.ovr"
save element nitrogen last "blr_fp89.nit"
save results last "blr_fp89.rlt"
save dr "blr_fp89.dr"
#
# blr_fp89.in
# class blr
# ======================================
```

Ferland and Persson (1989) presented this calculation of a BLR cloud. The differences between the present predictions and those given by FP are largely due to improved treatment of Balmer line escape and destruction. The spectrum is given relative to a Lya intensity of 100. The column density is VERY large, to reproduce intensities of low-ionization lines, especially the Ca II lines.

---

blr_hizqso.in

high Z quasar cloud

```
title high Z quasar cloud
#
# commands controlling continuum =========
table agn
ionization parameter 1
#
# commands for density & abundances =========
# actual elec den will be about 100x larger
hden 8
abundances starburst 35
#
# commands controlling geometry =========
# this is more gramage than it appears because of high Z
stop column density 21
#
# other commands for details =========
# once elec den fail occurs due to tripping over He+ - He I-front
# code does recover so not a problem. The default for this is 10,
# and is set low because (hopefully) this would never occur
# hydrogen is a minor constituent in this high metallicity gas
# the electron density is well above the hydrogen density
failures 3
iterate 3
#
# commands controlling output =========
normalize "blnd" 1909
save performance "blr_hizqso.per"
save dr "blr_hizqso.dr"
save convergence reason "blr_hizqso.cvr"
save overview last "blr_hizqso.ovr"
save element nitrogen last "blr_hizqso.nit"
save element chlorine last "blr_hizqso.cl"
save element iron last "blr_hizqso.fe"
save element neon last "blr_hizqso.ne"
save element calcium last "blr_hizqso.ca"
save element zinc last "blr_hizqso.zn"
save heating last "blr_hizqso.het"
save cooling last "blr_hizqso.col"
#
#
# blr_hizqso.in
# class blr
# ======================================
```

This is a model of a very high metallicty BLR cloud. It checks the intensities of some of the brigher lines, and is a check that the code can converge a cloud with this high Z.

Secondary ionization is very important when H is highly ionized, due to very high He abundance. Sec ionization becomes important at the He+ - He ionization front, where H+/H is 1e-5.

---

blr_kk81.in

old blr

```
title old blr
#
# commands controlling continuum =========
interpolate (0 -5) (.05 -5) (.1 0) (1 -0.5) (7.353 -2.233)
continue (735 -3.233) (800 -15) (8.e6 -15)
f(nu) -7.32148
constant gas pressure
#
# commands for density & abundances =========
hden 9.60206
init file="c84.ini"
abundances he=-1 c=-3.699 n=-4 o=-3.1549 ne=-4 na=-8 mg=-4.5229
continue al=-10 si=-4.4229 s=-10 ar=-10 ca=-10 fe=-4.5229 ni=-8
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
failures 2
iterate to convergence
#
# commands controlling output =========
print line faint -1
print ages
normalize "H 1" 1215.67A 100
save performance "blr_kk81.per"
save overview last "blr_kk81.ovr"
save convergence reason last "blr_kk81.cvr"
save dr last "blr_kk81.dr"
save continuum last "blr_kk81.con"
save ionizing continuum "blr_kk81.ion"
#
#
# blr_kk81.in
# class blr
# ======================================
#
```

This is the "standard" BLR model presented by Kwan and Krolik (1981).

>>refer blr cloud Kwan, J., & Krolik, J. 1981, ApJ, 250, 478

Compare line intensities to previous versions of CLOUDY by entering into table on page Error! Bookmark not defined..

The code caution that the resulting total pressure was not constant is to be expected. The KK calculation assumed constant gas pressure, but internally generature line radiation pressure is significant. Because of this the sum of gas plus radiation pressure was not constant although the gas pressure was.

`blr_level2.in`

test dominant level2 lines

```
title test dominant level2 lines
#
# commands controlling continuum =========
table agn
ionization -2
#
# commands controlling geometry =========
stop column density 19
```

```
#
# commands for density & abundances =========
hden 10
element phosphorus abundance 0
#
# other commands for details =========
iterate
#
# commands controlling output =========
save performance "blr_level2.per"
save convergence reason last "blr_level2.cvr"
save overview "blr_level2.ovr"
save dr "blr_level2.dr"
#
# blr_level2.in
# class blr
# ======================================
```

This model checks predictions for the "level2" lines. These are lines that are normally very weak, have Opacity Project wavelengths, and g-bar collision strengths. Phosphorus is given a large abundance so that its level2 lines are significant.

---

blr_n09_p18.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p18.per"
save overview "blr_n09_p18.ovr" last
save dr "blr_n09_p18.dr" last
save convergence reason "blr_n09_p18.cvr"
#
# blr_n09_p18.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n09_p18_Z20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
```

```
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 9
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
print h-like hydrogen departure coefficients
save performance "blr_n09_p18_Z20.per"
save overview "blr_n09_p18_Z20.ovr"
save dr "blr_n09_p18_Z20.dr"
save convergence reason "blr_n09_p18_Z20.cvr"
save convergence error "blr_n09_p18_Z20.cve"
#
# blr_n09_p18_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

`blr_n09_p20.in`

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p20.per"
save overview "blr_n09_p20.ovr" last
save dr "blr_n09_p20.dr" last
save continuum units Angstroms "blr_n09_p20.con" last
save convergence reason "blr_n09_p20.cvr"
#
# blr_n09_p18.in
```

```
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n09_p20_Z20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
abundances starburst 20
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p20_Z20.per"
save overview "blr_n09_p20_Z20.ovr" last
save dr "blr_n09_p20_Z20.dr" last
save convergence reason "blr_n09_p20_Z20.cvr"
#
# blr_n09_p20_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

This simulation is optically thin in the Lyman continuum - no H ionization front is present. As a result it can be difficult to converge.

---

blr_n09_p22.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
```

```
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p22.per"
save overview "blr_n09_p22.ovr" last
save dr "blr_n09_p22.dr" last
save convergence reason "blr_n09_p22.cvr"
#
# blr_n09_p22.in
# class blr
# ======================================
```

This is one of the models that sample the LOC plane.

`blr_n09_p22_Z20.in`

BLR model, density 1e09 cm-3, flux of H-ion phots 1e22 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e22 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
abundances starburst 20
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p22_Z20.per"
save overview "blr_n09_p22_Z20.ovr" last
save dr "blr_n09_p22_Z20.dr" last
save convergence reason "blr_n09_p22_Z20.cvr"
save convergence base "blr_n09_p22_Z20.cvb"
save element iron "blr_n09_p22_Z20.fe"
# save line emissivities when there is significant ionization stratification
# some of these ions will not exist at the inner edge or even anywhere in the sim
# saving the emissivities should still work correctly though...
save line emissivity "blr_n09_p22_Z20.ems"
Fe21 142.281A
blnd 1666A
O 1 6300.30
He 1 6678.15A
blnd 1240A
end of lines
#
# blr_n09_p22_Z20.in
# class blr
# ======================================
```

This is one of the models that sample the LOC plane.

blr_n11_p20.in

BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 11
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n11_p20.per"
save convergence reason "blr_n11_p20.cvr"
save overview "blr_n11_p20.ovr" last
save dr "blr_n11_p20.dr" last
#
# blr_n11_p20.in
# class blr
# ========================================
#
```

This is one of the 5 models that sample the LOC plane.

---

blr_n11_p20_Z20.in

BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20

```
title BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 11
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
```

```
save performance "blr_n11_p20_Z20.per"
save cooling "blr_n11_p20_Z20.col"
save convergence reason last "blr_n11_p20_Z20.cvr"
save heating "blr_n11_p20_Z20.het"
save element calcium "blr_n11_p20_Z20.cal"
save overview "blr_n11_p20_Z20.ovr"
save dr "blr_n11_p20_Z20.dr"
save temperature history "blr_n11_p20_Z20.tem"
#
# blr_n11_p20_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

2010 dec 25 This sim obtains different results for Hb and Fe II with gcc and icc. This is because the sim is not fully converged. Robin's & Peter's notes follow. This will probably be trac ticket #191

results changed with trivial changes in the source - Peter's example follows; This is due to lack of convergence rather than a fundamental difference in physics r4426:

Fe 2 2400A 6.854 1.9161 Fe 2 6200A 6.827 1.8005 Fe 2 2500A 6.984 2.5834 Fe 2 2300A 7.101 3.3854 Fe 2 8900A 6.714 1.3899

r4427:

Fe 2 2400A 6.852 1.9092 Fe 2 6200A 6.923 2.2472 Fe 2 2500A 6.943 2.3504 Fe 2 2300A 7.161 3.8897 Fe 2 8900A 6.671 1.2574

Robin; OK, I ran for 10 iterations with an old vs. new test on the cooling -- no substantial differences were reported.

The ne does seem to wander around quite a bit deep in the model, rather than smoothly converge -- attached plot is for the last iterations 5 to 10 (i.e. from when the code declares convergence in the standard blr_... run onwards). Not so bad as the difference plot which Peter shows, but not great. The temperature convergence seems better.

Suggests to me this may be a problem with poor convergence criteria/hysteresis, with the collisional cooling change just being the butterfly.

there's also an unresolved drop in both ne and H+ around 8.5e11 cm in the first iteration, which might be worth trying to understand.

Peter: It looks like there is a small thermal front in this model near the outer edge, though I derive this only from eyeballing the Te plot. They are quite common in blr models. It would also be a partial explanation of the jerky behavior of the code: gas near such a front will be quite sensitive to changes in cooling and/or heating since the curves are nearly parallel. It is however still worthwhile asking whether we are exacerbating the problem by writing the cooling terms in atom_leveln() the way we do.

Robin: Yes, there is a temperature front exactly at the rear of the slab (it only appears in the later iterations).

email exhange on this was around 2010 dec 22 - 24

`blr_n12_p19.in`

BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1

```
title BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1
#
# commands for density & abundances =========
#
# commands controlling continuum =========
```

```
table agn
phi(h) 19
#
# commands controlling geometry =========
hden 12
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n12_p19.per"
save convergence reason last "blr_n12_p19.cvr"
save overview "blr_n12_p19.ovr" last
save dr "blr_n12_p19.dr" last
#
#
# blr_n12_p19.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

`blr_n12_p19_Z20.in`

BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1, Z=20

```
title BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 19
#
# commands for density & abundances =========
hden 12
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
failures 5
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n12_p19_Z20.per"
save convergence reason "blr_n12_p19_Z20.cvr"
save overview "blr_n12_p19_Z20.ovr" last
save dr "blr_n12_p19_Z20.dr" last
#
# blr_n12_p19_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p18.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 13
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
init "c84.ini"
no level2 lines
save performance "blr_n13_p18.per"
save overview "blr_n13_p18.ovr" last
save dr "blr_n13_p18.dr" last
save convergence reason "blr_n13_p18.cvr"
#
# blr_n13_p18.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p18_Z20.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
# extend stopping temperature to low values to cover full column density
#
# commands controlling continuum =========
phi(h) 18
table agn
#
# commands for density & abundances =========
hden 13
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
stop temperature 1000
#
# other commands for details =========
# this sim needs roughly 10 iterations to converge
```

```
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
# abort if too many failures occur - we want to pass this test
# failures 2
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p18_Z20.per"
save overview "blr_n13_p18_Z20.ovr" last
save overview "blr_n13_p18_Z20.ovr1"
save dr "blr_n13_p18_Z20.dr" last
save convergence reason "blr_n13_p18_Z20.cvr"
save heating "blr_n13_p18_Z20.het"
save cooling "blr_n13_p18_Z20.col"
#
#
# blr_n13_p18_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p22.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e22 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e22 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 13
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p22.per"
save convergence reason last "blr_n13_p22.cvr"
save overview "blr_n13_p22.ovr" last
save dr "blr_n13_p22.dr" last
#
# blr_n13_p22.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p22_Z20.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 13
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p22_Z20.per"
save convergence reason last "blr_n13_p22_Z20.cvr"
save overview "blr_n13_p22_Z20.ovr"
save dr "blr_n13_p22_Z20.dr"
save heating "blr_n13_p22_Z20.het"
save cooling "blr_n13_p22_Z20.col"
#
# blr_n13_p22_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

`blr_n14_p18.in`

BLR model, density 1e14 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#stop efrac 0.1
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
init "c84.ini"
```

```
no level2 lines
save performance "blr_n14_p18.per"
save overview "blr_n14_p18.ovr" last
save dr "blr_n14_p18.dr" last
save convergence reason "blr_n14_p18.cvr"
#
# blr_n14_p18.in
# class blr
# ======================================
```

---

blr_n14_p20.in

BLR model, density 1e14 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n14_p20.per"
save convergence reason last "blr_n14_p20.cvr"
save overview "blr_n14_p20.ovr" last
save dr "blr_n14_p20.dr" last
#
# blr_n14_p20.in
# class blr
# ======================================
```

---

blr_n14_p22.in

BLR model, density 1e14 cm-3, flux of H-ion phots 1e22 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e22 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
```

```
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n14_p22.per"
save convergence reason last "blr_n14_p22.cvr"
save overview "blr_n14_p22.ovr" last
save dr "blr_n14_p22.dr" last
#
# blr_n14_p22.in
# class blr
# ======================================
```

---

blr_nf84.in

early model of blr

```
title early model of blr
#
# commands controlling continuum =========
ionization parameter -1.92
power law -1 100 0.01
#
# commands for density & abundances =========
hden 9.5
init, file="ism.ini"
abundances cameron
stop lyman optical 6
#
# commands controlling geometry =========
#
# other commands for details =========
constant gas pressure
iterate to convergence
#
# commands controlling output =========
save performance "blr_nf84.per"
save overview last "blr_nf84.ovr"
save convergence reason last "blr_nf84.cvr"
save dr last "blr_nf84.dr"
save results last "blr_nf84.rlt"
#
# blr_nf84.in
# class blr
# ======================================
#
```

This is an example of a "conventional" BLR calculation. The parameters are similar to those of Table 1 of Netzer and Ferland (1984). Notice that the ratio of Lyalpha to Hbeta ratio is much larger than observed.

>>refer blr model Netzer, H., & Ferland, G. J. 1984, PASP, 96, 593

---

blr_nf84_45deg.in

early model of BLR, with illumination at 45 degree angle

```
title early model of BLR, with illumination at 45 degree angle
#
# commands controlling continuum =========
ionization parameter -1.92
power law -1 100 0.01
# this continuum is a beam coming in at 45 degrees
illumination angle 45 degrees
#
# commands for density & abundances =========
hden 9.5
abundances cameron
stop lyman optical 6
#
# commands controlling geometry =========
#
# other commands for details =========
init file "ism.ini"
constant gas pressure
iterate to convergence
#
# commands controlling output =========
save performance "blr_nf84_45deg.per"
save overview "blr_nf84_45deg.ovr"
save convergence reason last "blr_nf84_45deg.cvr"
save dr "blr_nf84_45deg.dr"
save results last "blr_nf84_45deg.rlt"
#
# blr_nf84_45deg.in
# class blr
# ========================================
#
```

This is an example of a "conventional" BLR calculation. The parameters are similar to those of Table 1 of Netzer and Ferland (1984). Notice that the ratio of Lyalpha to Hbeta ratio is much larger than observed.

>>refer blr model Netzer, H., & Ferland, G. J. 1984, PASP, 96, 593

`blr_rnfa.in`

table 1 of Rees et al. ApJ 347, 648

```
title table 1 of Rees et al. ApJ 347, 648
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 10
init file="c84.ini"
abundances he= -1 c= -3.328 n= -4.0088 o= -3.0809 ne= -4 na= -20
continue mg= -4.3768 al= -5.5686 si= -4.36653 s= -4.76955
continue ar= -5.4202 ca= -5.6383 fe= -4.4815 ni= -20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize "H 1" 1215.67A = 100
print line faint -1
save performance "blr_rnfa.per"
```

```
save overview last "blr_rnfa.ovr"
save convergence reason last "blr_rnfa.cvr"
save continuum last "blr_rnfa.con" units microns
save transmitted continuum last "blr_rnfa.trn" units rydbergs
save element nitrogen last "blr_rnfa.nit"
save dr last "blr_rnfa.dr"
save results last "blr_rnfa.rlt"
#
# blr_rnfa.in
# class blr
# ======================================
#
```

This is the lower density cloud computed in Rees et al. (1989). Table 1 of that paper lists the predictions, which were a mean of those of Hagai Netzer's ION and roughly version 76 of CLOUDY. The lines are generally still in good agreement with the predictions of that paper. In particular the changes in the line fluxes shown in Figure 1 of that paper are reproduced quite well.

`blr_rnfb.in`

table 1 of Rees et al. ApJ 347, 648

```
title table 1 of Rees et al. ApJ 347, 648
#
# blr model from
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 12
init file="c84.ini"
abundances he= -1 c= -3.328 n= -4.0088 o= -3.0809 ne= -4 na= -20
continue mg= -4.3768 al= -5.5686 si= -4.36653 s= -4.76955
continue ar= -5.4202 ca= -5.6383 fe= -4.4815 ni= -20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint -1
print line optical depths
save performance "blr_rnfb.per"
save overview last "blr_rnfb.ovr"
save convergence reason last "blr_rnfb.cvr"
save element nitrogen last "blr_rnfb.nit"
save dr last "blr_rnfb.dr"
save results last "blr_rnfb.rlt"
save line emissivity "blr_rnfb.ems"
H 1 4861.32A
blnd 8446
blnd 1304
end of lines
normalize "H 1" 1215.67A = 91.8
#
# blr_rnfb.in
# class blr
# ======================================
#
```

This is a very dense cloud, and was computed in Rees et al. (1989). Table 1 of that paper lists the predictions, which were a mean of those of Hagai Netzer's ION and roughly version 76 of CLOUDY. The lines are generally still in good agreement with the predictions of that paper. In particular the changes in the line fluxes shown in Figure 1 of that paper are reproduced quite well. The fluxes of Lya and Hb are not reproduced with great precision by this model because of changes in collision rates for hydrogen and especially the form of the escape probability function for subordinate lines. As Figure 1 of RNF showed the line intensities are very sensitive to density for these parameters.

---

chianti_all_cool.in

cooling of a collisionally ionized plasma

```
title cooling of a collisionally ionized plasma
#
# commands controlling continuum =========
cosmic rays, background
coronal 4 vary
grid 4 6 0.5 sequential
database chianti "CloudyChiantiAll.ini" levels max
species "Fe+" levels=all
#
# commands for density & abundances =========
hden 0
set eden 0
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
save overview "chianti_all_cool.ovr"
save performance "chianti_all_cool.per"
save grid "chianti_all_cool.grd" last no hash
save cooling "chianti_all_cool.col" last no hash
save emitted continuum "chianti_all_cool.con" units angstroms
#
```

---

chianti_fe_cool.in

cooling of a collisionally ionized plasma

```
title cooling of a collisionally ionized plasma
#
# commands controlling continuum =========
cosmic rays, background
coronal 4 vary
database stout print
database chianti "CloudyChiantiFe.ini" print
species "Fe+" levels=all
grid 4 6 0.5 sequential
#
# commands for density & abundances =========
hden 0
init "honly.ini"
element iron on
element iron abundance 0
set eden 0
#
# commands controlling geometry =========
```

```
stop zone 1
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
save overview "chianti_fe_cool.ovr"
save performance "chianti_fe_cool.per"
save grid "chianti_fe_cool.grd" last no hash
save cooling "chianti_fe_cool.col" last no hash
save emitted continuum "chianti_fe_cool.con" units angstroms
#
```

This tests the use of Chianti limited to Fe ions, and the Kurucz Fe III, IV, and V added by Matt Lykins

---

coll_coronal.in

model of active region of solar corona

```
title model of active region of solar corona
#
# commands controlling continuum =========
# temperature of corona
coronal equilibrium, 2.5e6 K
# assume the sun is a blackbody at 5770K
blackbody 5770 K
luminosity solar linear 1
#
# commands for density & abundances =========
hden log=10
#
# commands controlling geometry =========
# its height above photosphere and thickness
radius 11 thickness = 10
# the gas fully covers the center of symmetry
sphere
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "o 8" 18.9689A
save overview "coll_coronal.ovr"
save performance "coll_coronal.per"
save dr "coll_coronal.dr" last
save continuum "coll_coronal.con" last units angstroms
#
#
# coll_coronal.in
# class coronal
# ======================================
#
```

This is a rough model of the solar corona. The test checks that the coronal equilibrium commands work. The gas is predominantly collisionally ionized.

---

coll_heat_only.in

test code in limit where ONLY mechanical heating is present

```
title test code in limit where ONLY mechanical heating is present
```

```
#
# commands controlling continuum =========
no photoionization
blackbody 5000 STE
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
hextra -1.5
iterate
#
# commands controlling output =========
# this command must be tested somewhere
print cooling, zone 5
# output files
save performance "coll_heat_only.per"
save overview "coll_heat_only.ovr"
save heating "coll_heat_only.het"
save cooling "coll_heat_only.col"
save convergence reason "coll_heat_only.cvr"
save dr "coll_heat_only.dr"
save continuum "coll_heat_only.con" units angstroms
#
#
# coll_heat_only.in
# class coronal
# ========================================
```

This test is an optically thin collisionally ionized gas with no photoionization at all.

`coll_t3.in`

coronal equilibrium at 10^3 K

```
title coronal equilibrium at 10^3 K
#
# commands controlling continuum =========
coronal 3
# add component of cosmic rays to drive chemistry
cosmic ray background
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
stop temperature off
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
# this sim needs very precise convergence to get a reliable result
set eden convergence tolerance 1e-4
#
# commands controlling output =========
save performance "coll_t3.per"
save overview "coll_t3.ovr"
save continuum "coll_t3.con" units angstroms
save dominant rates "coll_t3.sulphur" "S"
save dominant rates "coll_t3.molh2" "H2"
```

```
save dominant rates "coll_t3.molh" "H"
#
#
# coll_t3.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities. This is one of a series of sims coll_t?.in which test ionization over a range of temperatures. This one, unlike the others, includes cosmic rays. Chemistry is important at this low temperature and the chemical network will collapse without a source of ionization. The cosmic rays provide this source of ionization.

---

coll_t3_grains.in

coronal equilibrium at 10^3 K, with grains to assist chemistry

```
title coronal equilibrium at 10^3 K, with grains to assist chemistry
#
# commands controlling continuum =========
coronal 1e3K
# add component of cosmic rays to drive chemistry
cosmic ray background
# >>chng 20 sep 19 test updated ISM abundances
abundances "ISM-HD20.abn"
set H2 Jura rate
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop zone 1
#
# commands for density & abundances =========
hden 4
#
# other commands for details =========
# this sim needs very precise convergence to get a reliable result
set eden convergence tolerance 1e-4
#
# commands controlling output =========
save performance "coll_t3_grains.per"
save overview "coll_t3_grains.ovr"
save continuum "coll_t3_grains.con" units angstroms
#
#
# coll_t3_grains.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities. This is one of a series of sims coll_t?.in which test ionization over a range of temperatures. This one, unlike the others, includes cosmic rays and grains. Chemistry is important at this low temperature and the chemical network will collapse without a source of ionization. The cosmic rays provide this source of ionization.

---

coll_t4.in

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
```

```
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# commands controlling output =========
save performance "coll_t4.per"
save overview "coll_t4.ovr"
save continuum "coll_t4.con" units angstroms
#
#
# coll_t4.in
# class coronal
# ======================================
```

this tests conditions of collisional equilibrium at low densities

---

`coll_t4_Z30.in`

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
metals 30
#
# commands controlling output =========
save performance "coll_t4_Z30.per"
save overview "coll_t4_Z30.ovr"
save continuum "coll_t4_Z30.con" units angstroms
#
#
# coll_t4_Z30.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities and high metallicity, where H-O CX will strongly affect ionization of H

This is the high Z mate to coll_t4.in

`coll_t5.in`

coronal equilibrium at 10^5 K

```
title coronal equilibrium at 10^5 K
#
# commands controlling continuum =========
coronal 5
#
# commands controlling geometry =========
stop column density 15
# test the luminosity case
radius 13
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
iterate
#
#
# commands controlling output =========
# normalize to strong HeII line
normalize to "He 2" 303.784A
save performance "coll_t5.per"
save overview "coll_t5.ovr"
save continuum "coll_t5.con" units angstroms
#
# coll_t5.in
# class coronal
# ======================================
```

This is a test collisional ionization equilibrium at 1e5 K.

---

coll_t6.in

coronal equilibrium at 10^6 K

```
title coronal equilibrium at 10^6 K
#
# commands controlling continuum =========
coronal 6
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "c 5" 40.2678A
# output files
save performance "coll_t6.per"
save overview "coll_t6.ovr"
save continuum "coll_t6.con" units angstroms
#
# coll_t6.in
# class coronal
# ======================================
```

This test is an optically thin collisionally ionized gas.

---

coll_t7.in

coronal equilibrium at 10^7 K

```
title coronal equilibrium at 10^7 K
#
# commands controlling continuum =========
coronal 7
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
#
normalize to "o 8" 18.9689A
# commands controlling output =========
save performance "coll_t7.per"
save overview "coll_t7.ovr"
save continuum "coll_t7.con" units angstroms
save cooling "coll_t7.col"
save each cooling last "coll_t7.cole"
save cooling each "coll_t7.cle"
#
# coll_t7.in
# class coronal
# ======================================
```

Test with only collisional ionization at a high temperature.

`dynamics_orion_flow.in`

Orion nebula blister with wind

```
title Orion nebula blister with wind
#
# commands controlling continuum =========
blackbody 40000
phi(h) 13.0
brems 6
phi(h) 10
#
# commands for density & abundances =========
hden 4
abundances hii region no grains
grains orion no qheat single
#
# commands controlling geometry =========
wind -7 km/s advection
# this accounts for matter beyond end of the model
double optical depths
sphere
stop AV 5
stop temperature linear 5
#
# other commands for details =========
iterate 4
magnetic field -4
cosmic rays background
# this has no effect on dynamics, but is to desaturate the lines as per flow
turbulence 8 km/sec no pressure
# try to speed up simulation without hurting dynamics
```

```
init "fast.ini"
# use Bakes & Tielens heating
set PAH Bakes
#
# commands controlling output =========
# want to print line intensities are surface brightness, per arcsec^2
print lines surface brightness arcsec
print line faint -1.5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "dynamics_orion_flow.per"
save overview "dynamics_orion_flow.ovr" no hash
save hydrogen 21 cm "dynamics_orion_flow.21cm" no hash
save dr "dynamics_orion_flow.dr" no hash
save continuum last "dynamics_orion_flow.con" units microns no hash
save pressure "dynamics_orion_flow.pre" no hash
save heating "dynamics_orion_flow.het" no hash
save cooling "dynamics_orion_flow.col" no hash
save molecules "dynamics_orion_flow.mol" no hash
save wind "dynamics_orion_flow.wnd" last
#
# dynamics_orion_flow.in
# class dynamics hii pdr
# ======================================
#
```

This is a model similar in spirit to the blister geometry H+ region model computed by Baldwin et al. (1991), but with a D-critical flow. Many physical processes have been disabled to make this simulationn faster. Grain physics is not done so the gas temperature is incorrect. The main purpose is to do a quick test of the dynamical flow with grain opacities included. The slow directory contains a full simulation of a flow like Orion.

`dynamics_veryfast.in`

very fast wind model

```
title very fast wind model
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 9
# this is a set of commands to speed up calc
init file "fast.ini"
#
# commands controlling geometry =========
stop thickness 8.4
# this is a subsonic wind with advection
wind velo -5 advection
#
# other commands for details =========
# absolutely no convergence problems should occur
failures 1
# this degrades the continuum resolution by factor of 3, to
# speed up calc
set continuum resolution 3
iterate 4
#
# commands controlling output =========
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "dynamics_veryfast.ovr"
save performance "dynamics_veryfast.per"
save pressure last "dynamics_veryfast.pre"
```

```
save total opacity last "dynamics_veryfast.opc"
save ionizing continuum last "dynamics_veryfast.ion"
save continuum last "dynamics_veryfast.con"
save dr "dynamics_veryfast.dr"
#
#
# dynamics_veryfast.in
# class dynamics
# ======================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

---

dynamics_veryfast_rec.in

very fast wind model

```
title very fast wind model
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 9
# this is a set of commands to speed up calc
init file "fast.ini"
#
# commands controlling geometry =========
stop thickness 8.4
# this is a subsonic wind with advection
wind velo 5 advection
#
# other commands for details =========
# absolutely no convergence problems should occur
failures 1
# this degrades the continuum resolution by factor of 3, to
# speed up calc
set continuum resolution 3
iterate 4
#
# commands controlling output =========
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "dynamics_veryfast_rec.ovr"
save performance "dynamics_veryfast_rec.per"
save pressure last "dynamics_veryfast_rec.pre"
save total opacity last "dynamics_veryfast_rec.opc"
save ionizing continuum last "dynamics_veryfast_rec.ion"
save continuum last "dynamics_veryfast_rec.con"
save dr "dynamics_veryfast_rec.dr"
#
#
# dynamics_veryfast_rec.in
# class dynamics
# ======================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

---

dynamics_wind.in

test of equations of motion in a very highly ionized wind

```
title test of equations of motion in a very highly ionized wind
#
# test motion in electron scattering limit
# radiative acceleration (e- only) is 9.54E-7 cm s^-2
# terminal velocity (e- only) is 7.6 km s^-1
#
# commands controlling continuum =========
table agn
luminosity (total) 45
#
# commands for density & abundances =========
hden 4
# this only includes H and He
init file="hheonly.ini"
#
# commands controlling geometry =========
radius (parsecs) 1
stop thickness (parsecs) -1
# a slow wind velocity, will assert velocity at outer radius
wind velo 0.1 ball
#
# other commands for details =========
# this will speed things up a bit
no level2
no radiation pressure
constant temperature 8
#
# commands controlling output =========
save overview "dynamics_wind.ovr"
save performance "dynamics_wind.per"
save pressure "dynamics_wind.pre"
save wind "dynamics_wind.wnd"
save dr "dynamics_wind.dr"
#
# dynamics_wind.in
# class limit dynamics
# ======================================
#
```

This tests the radiative acceleration and terminal velocity of a wind in which only electron scattering is important. The parameters were chosen so that electron scattering is the dominant opacity source, so that the equations can be solved both numerically (in the example) and analytically (the expected solution given above). In a realistic wind the gas would be more neutral and line driving would dominate. The force multiplier, given in the save wind output, is nearly unity as a result.

Checks:
- The radiative acceleration is correct (e- 9.543910-7 cm s-2).
- The terminal velocity should be 7.57 km s-1.
- Force multiplier near unity (no line driving since so highly ionized).
- Thickness of cloud correct (R-Ro + dr/2 should be 3.086391017 cm).

`feii_hin.in`

test feii in high density limit

```
title test feii in high density limit
#
# commands controlling continuum =========
black 25000 K
```

```
ionization -10
#
# commands for density & abundances =========
hden 18
# force a high electron density to insure collisions dominate
eden 18
#
# commands controlling geometry =========
constant tempera 4
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
iterate
# want to test collision only limit
no induced processes
#
# commands controlling output =========
set save prefix "feii_hin"
save overview ".ovr"
save performance ".per"
save species continuum ".fe2con" "Fe+" last units microns
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
# feii_hin.in
# class limit
# ======================================
#
```

This checks that, at high particle densitites, in which the gas should be in collisional equilibrium, the level populations of the large model Fe+ ion go to the proper values, where the departure coefficients are all equal to unity.

`feii_hirad.in`

feii in case of high radiation density limit

```
title feii in case of high radiation density limit
#
# commands controlling continuum =========
black 8000 K lte
#
# commands for density & abundances =========
hden 9
element iron abundance 2
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
constant tempera 8000
iterate
#
# commands controlling output =========
set save prefix "feii_hirad"
save overview ".ovr"
save performance ".per"
save species densities ".lv1" "Fe+[:200]" last
save species densities ".lv2" "Fe+[201:]" last
save species continuum ".fe2con" "Fe+" last units microns
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
```

```
# feii_hirad.in
# class limit
# ======================================
#
```

This checks that, at high radiation densitites, in which the gas is irradiated by a blackbody in strict thermodynamic equilibrium, the level populations of the large model Fe+ ion go to the proper values, where the departure coefficients are all equal to unity.

`feii_pump.in`

test feii in continuum pumped limit

```
title test feii in continuum pumped limit
#
# commands controlling continuum =========
black 25000 K
ionization -5
#
# commands for density & abundances =========
hden 10
abundances old solar 84
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
Case B
iterate
constant tempera 4
species "Fe+" levels=all
#
# commands controlling output =========
set save prefix "feii_pump"
save overview ".ovr"
save performance ".per"
save species continuum ".con" "Fe+" units microns last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
# feii_pump.in
```

This is a constant temperature low ionization cloud, with BLR-like densities, which includes the large FeII atom. The tests check on the emission predicted in the Fe II bands.

This model tests the large FeII model in the optically thin, continuum pumped limit. The zone thickness is set to a small value (1 cm) so that full continuum hits atom.

`feii_ste.in`

thermal equilibrium of FeII in STE limit

```
title thermal equilibrium of FeII in STE limit
#
# commands controlling continuum =========
black 8000 K lte
hden 9
#
# commands for density & abundances =========
element iron abundance 2
```

```
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
iterate
#
# commands controlling output =========
set save prefix "feii_ste"
save overview ".ovr"
save performance ".per"
save continuum last ".con"
save species column density last ".col" "Fe+"
save species densities last ".pop" "Fe+[:]"
save species departure last ".dep" "Fe+[:]"
save species levels last ".lev" "Fe+"
save species continuum ".fe2con" "Fe+" last units microns
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
# feii_ste.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. It is irradiated by a blackbody in strict thermodynamic equilibrium. We check that the temperature of the gas is equal to the radiation temperature, to confirm that the thermal properties of the model FeII atom obey thermodynamics.

`feii_t4n0.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 0
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n0"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
```

```
#
# feii_t4n0.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

`feii_t4n8.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

`feii_t4n8_rt.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop thickness 5
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
iterate 3
#
# commands controlling output =========
print line precision 6
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_rt"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species inward continuum last ".cin" "Fe+" units angstroms
save species outward continuum last ".cout" "Fe+" units angstroms
save species column density last ".col" "Fe+[:]"
save species densities last ".pop" "Fe+[:]"
save species optical depth last ".opt" "Fe+"
save species lines last ".lin" "Fe+"
save species bands ".fe2b" "FeII_bands.dat" "Fe+"
save line emissivity ".ems"
"Fe 2b" 2797
"InwdBnd" 2797
end of lines
#
#
# feii_t4.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has intermediate density and should produce and FeII spectrum something like an AGN. The set line precision 6 increases the number of significant figures in the wavelengths for each line. This is needed to get the right FeII inward band.

This has a finite thickness and so tests the RT, line overlap.

`feii_t4n8_Smyth19.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Smyth19"
database Stout print
#
# commands controlling continuum =========
black 5e5K
```

```
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Smyth19"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ========================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

`feii_t4n8_Tayal18.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Tayal18"
database Stout print
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
```

```
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Tayal18"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

`feii_t4n8_Verner99.in`

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Verner99"
database Stout print
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Verner99"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

`func_abund_fluc.in`

check fluctuating heavy-element abundances

```
title check fluctuating heavy-element abundances
# commands controlling continuum =========
blackbody 5
ionization -2
#
# commands for density & abundances =========
hden 3
# this varies the abundnaces between default and 1e-4 times default,
# over a 1e10 cm period - we will compute half a cycle
fluctuations abundances 10.3 0 -4
#
# commands controlling geometry =========
# stop at half a cycle so pick off lowest abundances
stop thickness 10
#
# other commands for details =========
# speed things up a bit
init "c84.ini"
#
# commands controlling output =========
print column density
save performance "func_abund_fluc.per"
save overview "func_abund_fluc.ovr"
save abundances "func_abund_fluc.abn"
#
# commands giving asserts
#
# func_abund_fluc.in
# class function
# ======================================
#
```

This checks that the variable abundances option works

`func_distance.in`

check that distance and "print flux earth" commands work

```
title check that distance and "print flux earth" commands work
#
# commands controlling continuum =========
# luminosity in ionizing radiation, this and distance
# were chosen so that flux at earth assocated with total
# luminoisity of object is 1 erg cm-2 s-1
luminosity 40
laser 2
#
# must test capabiliites somewhere
# >>19 07 09, add abundances
abundances "palme14-Sol.abn"
#
# commands for density & abundances =========
```

```
hden 4
# >>19 07 09, add abundances
# init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
radius 17
#
# other commands for details =========
distance 19.450395
constant temperature 4
#
# commands controlling output =========
# give flux at Earth
print lines, flux at Earth
save overview "func_distance.ovr"
save performance "func_distance.per"
#
# func_distance.in
# class function
# ======================================
#
```

Normally the code predicts the intensity or luminosity of the emission lines. This test confirms that it can predict the flux recieved at the Earth instead. The model is the simplest and fastest that can be computed - a H-only constant temperature single zone. The total luminosity is set to 1e40 erg/s, and the ionization source is a laser at 2 ryd. With these set, the total luminosity in ionizing radiation, the total luminoisity in the incident continuum (the emission line labeled "Inci 0") will be 1e40.

The code will predict the flux at the Earth if both the distance to the oject is specified with the distance command, and this is requested with the print flux earth command. The distance was chosen so that the total flux at the Earth will be 1 erg/s. This is asserted at the end of the calculation.

`func_dlaw.in`

test model with dlaw table

```
title test model with dlaw table
#
# commands controlling continuum =========
phi(H) 15
table agn
#
# commands for density & abundances =========
dlaw table radius
continue 16 9
continue 17 7
continue 18 5
continue 19 3
continue 20 1
continue 21 -1
end of dlaw
#
# must test capabiliites somewhere
# >>19 07 09, add abundances
abundances "palme14-Met.abn"
#init "honly.ini"
#
# commands controlling geometry =========
sphere
filling factor -5
radius 17 20
#
# other commands for details =========
```

```
constant temperature 4
#
# commands controlling output =========
save overview "func_dlaw.ovr"
save performance "func_dlaw.per"
save dr "func_dlaw.dr"
save overveiw "func_dlaw.ovr"
#
#
# func_dlaw.in
# class function
# ======================================
#
```

this model tests the dlaw density table command

`func_fulltrace.in`

test full trace output

```
title test full trace output
#
# commands controlling continuum =========
trace h-like hydrogen full no print
# check that no uninitialized rates are printed (r2757)
print arrays ionization carbon only
print arrays levels "C[1:5]"
stop zone 1
table agn
ionization parameter -0.5
#
# commands for density & abundances =========
hden 9.5
init file="honly.ini"
element carbon on
#
# other commands for details =========
database h-like element hydrogen collapsed levels 1
#
# commands controlling output =========
# func_fulltrace.in
# class function
# ======================================
```

this checks that trace output functions correctly

`func_globule.in`

test of globule command

```
title test of globule command
#
# commands controlling continuum =========
black 40000 K
ionization parameter -1.5
#
# commands for density & abundances =========
globule initial density=5 scale depth=14
init file "ism.ini"
abundances hii region no qheat
#
```

```
# commands controlling geometry =========
#
# other commands for details =========
failures 2
#
# commands controlling output =========
print line faint -1.5
save performance "func_globule.per"
save overview last "func_globule.ovr"
save results last "func_globule.rlt"
save dr "func_globule.dr" last
save heating "func_globule.het" last
save cooling "func_globule.col" last
#
# func_globule.in
# class function
# ======================================
#
```

This model uses the globule command, tests that the zoning logic works for this extreme case, and that the code is able to converge the globule model.

`func_grid_line_ratios.in`

test generating line ratios in a grid run

```
title test generating line ratios in a grid run
#
# commands controlling continuum =====
blackbody 4e4 K
ionization parameter -2
#
# commands for density & abundances =====
# these are to speed up the calculation, only do H, O, and Ne
init "honly.ini"
element oxygen on
element neon on
element sulphur on
element oxygen ionization 1 1 1
element neon ionization 1 1 1
element sulphur ionization 1 1 1
# vary the hydrogen density
hden 4 vary
grid 2 6.1 1 sequential
#
# other commands for details =======
# these are constant temperature models, vary T
constant temperature 4 vary
grid 4000 17000 3000 linear
stop zone 1
#
# commands controlling output =====
save overview "func_grid_line_ratios.ovr"
save performance "func_grid_line_ratios.per"
save line list "func_grid_line_ratios.pun" "func_grid_line_ratios.dat" ratio no hash
save grid "func_grid_line_ratios.grd"
#
# commands giving (lack of) assert ==========
#
# func_grid_line_line_ratios.in
# class function
# ================================================
```

This uses the grid command to compute line ratios for a wide range of density and temperature. The ionization is set to a uniform value and only a few elements are included. this makes the calculation faster and prevents recombination [O III]

4363 from becoming important (there is no O+3).

These are the line ratios mentioned as limits in the Johnstone et al. Spitzer cooling flow filament paper (2007).

`func_grid_list.in`

test the 'list' keyword on the grid command

```
title test the 'list' keyword on the grid command
blackbody 10000 STE vary
grid list "func_grid_list.dat" linear sequential
hden 5
stop zone 1
iterate 2
****************
```

This is a simple grid with parameter values stored in an external file. That file is also used to monitor the temperature of each grid point.

`func_hotgas_coolstar.in`

test very soft continuum, very hot gas

```
title test very soft continuum, very hot gas
#
# commands controlling continuum =========
# put in the cosmic background as the only continuum source
CMB
# gas has constant temperature of 1e6 K
constant temperature, t=6
#
# commands for density & abundances =========
hden 10.
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas - 1 cm thick
set dr 0
#
# other commands for details =========
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_hotgas_coolstar.ovr"
save performance "func_hotgas_coolstar.per"
#
# func_hotgas_coolstar.in
# class limit
# ======================================
#
```

This is a test where the CMB is the only continuum source. It does not extend to energies where the code needs to work. There are special cases used in this situation, for continuum addressing, so this checks whether those still function.

`func_ion_increase.in`

test model where ionization increases with depth

```
title test model where ionization increases with depth
#
# commands controlling continuum =========
ionization parameter -4
table agn
#
# commands for density & abundances =========
hden 7 -4
init "hheonly.ini"
element oxygen on
element iron on
#
# commands controlling geometry =========
sphere
filling factor -5
radius 17 20
#
# other commands for details =========
constant temperature 4
#
# commands controlling output =========
save overview "func_ion_increase.ovr"
save performance "func_ion_increase.per"
save dr "func_ion_increase.dr"
save overveiw "func_ion_increase.ovr"
save element oxygen "func_ion_increase.oxy"
save element iron "func_ion_increase.fe"
#
#
# func_ion_increase.in
# class function
# ========================================
#
```

This density falls off faster than 1/r^2 so the ionization increases with depth. Most sims have decreasing rather than increasing ionization.

`func_iso_large.in`

test large iso sequence model atom

```
title test large iso sequence model atom
#
# commands controlling continuum =========
blackbody 5e4
ionization parameter -2
CMB
#
# commands for density & abundances =========
hden = 2.3
eden = 2.3
metals .3 log
#
# commands controlling geometry =========
sphere
stop zone 10
#
# other commands for details =========
database H-like levels large element hydrogen
database He-like levels large element helium
#
```

```
# commands controlling output =========
print every 1
database H-like levels print
save performance "func_iso_large.per"
save dr "func_iso_large.dr"
save overview "func_iso_large.ovr"
save line labels "func_iso_large.lbl"
#
#
# func_iso_large.in
# class function
# ======================================
#
```

this model tests the large model atoms for the iso sequences. the large models are used for H I and He I. monitor lines from both low-lying and Rydberg levels to test the full model. the lines from Rydberg states as well as the He I 10830 line are ambiguous so this also exercises line disambiguation

---

func_LineList_BLR.in

```
test
print line precision 6
table lines "LineList_BLR.dat"
```

---

func_LineList_BLR_Fe2.in

```
test
print line precision 6
table lines "LineList_BLR_Fe2.dat"
set save prefix "func_LineList_BLR_Fe2"
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
```

---

func_LineList_BLR_Fe2_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_BLR_Fe2.dat"
set save prefix "func_LineList_BLR_Fe2"
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
```

---

func_LineList_BLR_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_BLR.dat"
```

---

func_LineList_He_like.in

```
test
print line precision 6
table lines "LineList_He_like.dat"
```

---

func_LineList_He_like_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_He_like.dat"
```

---

func_LineList_HeH.in

```
test
print line precision 6
table lines "LineList_HeH.dat"
```

---

func_LineList_HeH_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_HeH.dat"
```

---

func_LineList_HII.in

```
test
print line precision 6
table lines "LineList_HII.dat"
```

---

func_LineList_HII_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_HII.dat"
```

---

func_LineList_NLR.in

```
test
print line precision 6
table lines "LineList_NLR.dat"
```

---

func_LineList_NLR_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_NLR.dat"
```

---

func_LineList_PDR.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
print line precision 6
table lines "LineList_PDR.dat"
```

---

func_LineList_PDR_H2.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
database h2
print line precision 6
table lines "LineList_PDR_H2.dat"
```

---

func_LineList_PDR_H2_vacuum.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
database h2
print line precision 6
print lines vacuum
table lines "LineList_PDR_H2.dat"
```

---

func_LineList_PDR_vacuum.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
print line precision 6
print lines vacuum
table lines "LineList_PDR.dat"
```

---

func_LineList_strong.in

```
test
print line precision 6
table lines "LineList_strong.dat"
```

---

func_LineList_strong_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_strong.dat"
```

---

func_lines.in

create output file with list of func_lines

```
title create output file with list of func_lines
print line precision 6
database h2 levels large
species "Fe+" levels=all
# report all species in use
database print
test
#
# commands controlling continuum =========
# commands for density & abundances =========
# commands controlling geometry =========
# other commands for details =========
#
# commands controlling output =========
# this creates the file "func_lines.lab" that contains a list
# of all emission labels
save overview "func_lines.ovr"
save performance "func_lines.per"
save line labels "func_lines.lab"
# the save species xxx series of line-related reports
save species labels "func_lines.spclab" all
save species lines "func_lines.spclin" all
save species levels units wavenumber "func_lines.spclev" all
# this must come last since code stops after doing it
# this creates the file "func_lines.lis" that contains a list
# of the emission func_lines that are transported.
save line data "func_lines.lis"
#
# There is nothing extra to assert, since test does include many asserts
#
# func_lines.in
# class function
# ======================================
#
```

This runs the standard "test" case, and then creates the line data and labels files. Test by itself includes many asserts, so no further asserts are needed here.

The file func_lines.lab is a useful list of all lines predicted by the code. Cut and paste this into other places when you need to find a particular emission line.

The func_lines lines.dat gives atomic data for all the lines, and their critical density at 10000 K. The large H2 and Fe II model atoms are turned on to include their lines.

---

func_ly_pump_scale.in

test scaling of H lyman-line pumping

```
title test scaling of H lyman-line pumping
sphere
blackbody 30000
q(h) 47
hden 2.5
radius 16
stop zone 1
database H-like Lyman pumping scale .2
```

This purpose of this test is just to exercise the option to scale the H lyman series pumping rates by some factor.

`func_map.in`

map of heating vs cooling

```
title map of heating vs cooling
#
# commands controlling continuum =========
table agn
ionization parameter -2.5
#
# commands for density & abundances =========
hden 0
abundances old solar 84
#
# commands controlling geometry =========
set dr 0
stop lyman optical depth -7
stop zone 1
#
# other commands for details =========
#
# commands controlling output =========
# save map information to generate plot for hazy
save overview "func_map.ovr"
save performance "func_map.per"
save map file="func_map.dta"
set nmaps 100
#
# map.in
# class function
# ======================================
#
```

This is a test of the continuity of the code over a very large range of temperature. It was used to produce one of the thermal maps shown in Hazy.

Checks:
- No breaks in the heating and cooling curves where various approximations change.

`func_nolight.in`

check OK with no radiation incident

```
title check OK with no radiation incident
constant temp 5e7 linear
hden 7 log
set dr 0
stop zone 1
#
save performance "func_nolight.per"
save dr "func_nolight.dr"
save overveiw "func_nolight.ovr"
#
#
# func_nolight.in
# class function
```

```
# ======================================
#
```

Check that we handle limit where there is no incident radiation field

---

`func_sdrmin.in`

test set drmin command

```
title test set drmin command
#
# commands controlling continuum =========
blackbody 8e4
luminosity 37.5
#
# commands for density & abundances =========
hden 4
#
# commands controlling geometry =========
radius 17
sphere
stop thickness 17.03
stop temperature off
#
# other commands for details =========
set drmin 15.5
cosmic rays background
#
# commands controlling output =========
save overview "func_sdrmin.ovr"
save performance "func_sdrmin.per"
save dr "func_sdrmin.dr" last
#
```

This simulation tests the SET DRMIN command. It is a toy model of a planetary nebula that is designed to extend into the PDR. The minimum stepsize is deliberately set much too large so that we would immediately notice if the command was broken. It also tests if we still hit the correct outer radius when SET DRMIN is used. Without the SET DRMIN command this sim would need 410 zones (trunk@2760).

`func_set_ion.in`

test impact of setting ionization

```
title test impact of setting ionization
#
# commands for density & abundances =========
init "ism.ini"
hden 0
element hydrogen ionization 0 1
element helium ionization 0 1 0
element carbon ionization 0 1
element oxygen ionization 0 0.1 0.2 0.3 0.2 0.1 0.1
element iron ionization -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 0 -9 -9
#
# commands controlling continuum =========
blackbody 5
ionization parameter -2
#
# commands controlling geometry =========
# force model to be 1 cm thick
```

```
set dr 0
#
# other commands for details =========
constant temperature 4
stop zone 1
#
# commands controlling output =========
#>>chng 23 oct 13 add this command to test somewhere in tsuite
print lines vacuum
normalize to "o 3" 5006.84 air
save overview "func_set_ion.ovr"
save performance "func_set_ion.per"
save dr "func_set_ion.dr"
#
#
# func_set_ion.in
```

class function # ========== # this script exercies the option to specify the ionization of a species

---

func_stopcol.in

test stop column density "species" command

```
title test stop column density "species" command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
init file "ism.ini"
# test option to turn off elements with small abundances
element limit off -5
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop column density "N+2" 10.
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
set save prefix "func_stopcol"
save overview ".ovr"
save performance ".per"
save dr ".dr" last
#
#
#
#
# func_stopcol.in
# class function
# ========================================
#
```

This is an example of a simple calculation that stops when a column density of a species reaches a specific value. The tricky part is that the species label contains a number, so we need to ascertain that the column density is parsed correctly.

---

func_stopline1.in

test stop line command

```
title test stop line command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
abundances old solar 84
init file "ism.ini"
# test option to turn off elements with small abundances
element limit off -5
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop line "c 2" 157.636m reaches 0.0358
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
save overview "func_stopline1.ovr"
save performance "func_stopline1.per"
save dr "func_stopline1.dr" last
#
# func_stopline1.in
# class function
# ======================================
#
```

This is an example of a simple calculation that stops when a line reaches a specified intensity. The option to turn off elements with trivial abundances is used.

`func_stopline2.in`

test stop line command

```
title test stop line command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
abundances old solar 84
init file "ism.ini"
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop line "c 2" 157.636m air reaches 0.002 relative to "o 3" 5008.24 vacuum
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
normalize to "o 3" 5006.84
save overview "func_stopline2.ovr"
save performance "func_stopline2.per"
save dr "func_stopline2.dr" last
#
```

```
# func_stopline2.in
# class function
# ======================================
#
```

this is an example of a simple calculation that stops when a certain emission line ratio is reached

---

`func_t10.in`

test very soft continuum, very hot gas

```
title test very soft continuum, very hot gas
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden 1.
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas - 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to high-T limit
constant temperature, t=10 log
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_t10.ovr"
save performance "func_t10.per"
#
#
# func_t10.in
# class limit
# ======================================
#
```

This is a test of the highest temperature the code can do.

`func_t3.in`

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
```

```
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_t3.ovr"
save performance "func_t3.per"
#
#
#
# func_t3.in
# class limit
# ======================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K

`func_t3_linesintroff.in`

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
print lines intrinsic off
set save prefix "func_t3_linesintroff"
save overview ".ovr"
save performance ".per"
#
#
#
# func_t3.in
# class limit
# ======================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K. The predicted intrinsic spectrum is suppressed in the main output.

`func_t3_linesoff.in`

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
print lines off
set save prefix "func_t3_linesoff"
save overview ".ovr"
save performance ".per"
#
#
#
# func_t3.in
# class limit
# ======================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K. The predicted spectra (intrinsic and emergent) are suppressed in the main output.

`func_test.in`

run smoke test

```
title run smoke test
# commands controlling continuum =========
test
# commands for density & abundances =========
# commands controlling geometry =========
# other commands for details =========
# include this in one test to make sure it works
set continuum shield ferland
#
# commands controlling output =========
# increase precision of all printed wavelengths
print line precision 6
# following will print physical constants used by the code
print constants
# print RR and DR rates
print recombination
# print the past to the data directory
print path
# the citation for the current version of the code
print citation
# following prints column densities
print column density
save performance "func_test.per"
save continuum "func_test.con"
```

```
save overview "func_test.ovr"
# func_test.in
# class function
# ======================================
#
```

This runs the smoke test command, which include several asserts. The tests the behavior of increasing the number of significant figures in printed wavelengths.

---

func_test_cycle.in

exercise full range of density, temperature

```
title exercise full range of density, temperature
#
# modified from slow/grid_extreme.in
# this version cycles through the corner models twice
# to see if the second repetition exactly matches the first
# checkall.pl calls test_grid.pl to check that output is identical
#
element lithium off
element berylium off
element boron off
cosmic rays background linear 0.1266
cmb
iterate
#
blackbody 6
energy density 6 vary
grid 1 6 5 cycle sequential
# -8 18
hden 2 vary
grid -6 15 21
stop zone 1
# set to constant small thickness
set dr -10
#
trace h-like full helium no print
trace he-like full no print
trace heavy no print
trace convergence esource no print
no time
#
save performance no hash "func_test_cycle.per"
save grid no hash "func_test_cycle.grd" last
save overview last no hash "func_test_cycle.ovr" last
save average "func_test_cycle.avr" last
temperature hydrogen 2
end of average
#
#
# func_test_cycle.in limits
```

---

func_test_grid.in

test whether the output from a repeated model reproduces exactly

```
title test whether the output from a repeated model reproduces exactly
print depart he-like element helium
trace h-like full helium no print
trace he-like full no print
```

```
trace heavy no print
trace convergence esource no print
test
no time
fudge 0 vary
grid 0 to 1 1 repeat sequential
iterate 3
***************
```

This tests that the code gets repeatable results in a large grid run. It will not if variables are not properly initialized. tsuite / programs / comp does a similar test.

auto / checkall.pl includes test to check this.

`func_testmole.in`

this runs the standard, one command, test, which contains many asserts

```
title this runs the standard, one command, test, which contains many asserts
# commands controlling continuum =========
test mole
#
# commands for density & abundances =========
# commands controlling geometry =========
# other commands for details =========
#
# commands controlling output =========
save performance "func_testmole.per"
save overview "func_testmole.ovr"
# func_testmole.in
# class function
# ======================================
#
```

This runs the "test mole" command, which include several asserts.

`func_tlaw.in`

test model with tlaw table

```
title test model with tlaw table
#
# commands controlling continuum =========
phi(H) 15
table agn
#
# commands for density & abundances =========
hden 9
init "honly.ini"
#
# commands controlling geometry =========
sphere
filling factor -5
radius 16 17
stop temperature 3 linear
#
# other commands for details =========
tlaw table radius
continue -35 4
continue 16 4
continue 16.2 3
```

```
continue 16.4 4
continue 16.6 3.5
continue 16.8 4
continue 20 4
continue 21 -1
end of tlaw
#
# commands controlling output =========
save overview "func_tlaw.ovr"
save performance "func_tlaw.per"
save dr "func_tlaw.dr"
save overveiw "func_tlaw.ovr"
#
#
# func_tlaw.in
# class function
# ======================================
#
```

this model tests the tlaw density table command

---

func_trans_lumi.in

test transmitted continuum in luminosity mode

```
title test transmitted continuum in luminosity mode
#
# common commands
init file "func_trans_lumi.dat"
#
# commands controlling geometry =========
radius 21
#
# commands controlling output =========
set save prefix "func_trans_lumi"
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
#
# this contains a large number of asserts that both tests use
init file "trans_lumi.dat"
#
# func_trans_lumi.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

---

func_trans_read.in

second of func_trans_save/func_trans_read pair, use transmitted continuum

```
title second of func_trans_save/func_trans_read pair, use transmitted continuum
# the transmitted continuum produced by func_trans_punch
#
# commands controlling continuum =========
ionization parameter -1
table read "func_trans_save.trn"
brems 6
ionization parameter -6
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
# this contains a large number of asserts used by both commands
init file "trans.dat"
save overview "func_trans_read.ovr"
save performance "func_trans_read.per"
save ionization last "func_trans_read.ion"
#
#
# func_trans_read.in
# class function
# ======================================
#
```

func_trans_save.in and func_trans_read.in are a pair of tests that check that the code can save a transmitted continuum then read it.

`func_trans_read_lumi_scale.in`

test read transmitted continuum in luminosity mode

```
title test read transmitted continuum in luminosity mode
#
# commands controlling continuum =========
table read "func_trans_save_lumi.trn" scale
# second, very faint SED to force luminosity mode
blackbody 50
luminosity 1
#
# commands for density & abundances =========
hden 3
#
# commands controlling geometry =========
radius 21
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
set save prefix "func_trans_read_lumi_scale"
```

```
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
#
# this contains a large number of asserts that both tests use
init file "trans_lumi.dat"
#
# func_trans_read_lumi_scale.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

This sim must come after func_trans_save_lumi since it needs the save file generated by func_trans_save_lumi.

`func_trans_read_scale.in`

second of func_trans_save/func_trans_readread pair

```
title second of func_trans_save/func_trans_readread pair
# use the transmitted continuum produced by func_trans_save
#
# commands controlling continuum =========
# 10 continua scaled to 1/10 original should get same answer
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
# this contains a large number of asserts used by both commands
init file "trans.dat"
save overview "func_trans_read_scale.ovr"
save performance "func_trans_read_scale.per"
```

```
save ionization last "func_trans_read_scale.ion"
# transmitted continuum should scale as specified
save last transmitted continuum "func_trans_read_scale.trn"
#
#
# func_trans_read_scale.in
# class function
# ========================================
#
```

func_trans_save.in and func_trans_read_scale.in are a pair of tests that check that the code can save a transmitted continuum then read it.

`func_trans_save.in`

first of func_trans_save/func_trans_read pair, save continuum

```
title first of func_trans_save/func_trans_read pair, save continuum
#
# commands controlling continuum =========
ionization parameter -1
table agn
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "func_trans_save.ovr"
save performance "func_trans_save.per"
save ionization last "func_trans_save.ion"
save continuum last "func_trans_save.con"
# this continuum will be used by transread.in
save last transmitted continuum "func_trans_save.trn"
#
# this contains a large number of asserts that both tests use
init file "trans.dat"
#
# func_trans_save.in
# class function
# ========================================
#
```

func_trans_save, func_trans_read, func_trans_read_scale are a set of tests that check that the code can save a transmitted continuum then read it.

This sim must come before func_trans_read since it generates the save file needed by func_trans_read. Alphabetical order insures this.

`func_trans_save_lumi.in`

test save transmitted continuum in luminosity mode

```
title test save transmitted continuum in luminosity mode
```

```
#
# common commands
init file "func_trans_lumi.dat"
#
# commands controlling geometry =========
radius 20
#
# commands controlling output =========
set save prefix "func_trans_save_lumi"
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
save transmitted continuum ".trn"
#
#
# func_trans_save_lumi.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

This sim must come before func_trans_read_lumi_scale since it generates the save file needed by func_trans_read_lumi_scale.

`grains_hot.in`

test temperature of gas and dust in high energy density environment

```
title test temperature of gas and dust in high energy density environment
#
# commands controlling continuum =========
table power law
# intensity of incident radiation field set by its energy density
energy density temp 550 K
#
# commands for density & abundances =========
hden 5.0
init "ism.ini"
# Orion grains and abundances
abundances orion
#
# commands controlling geometry =========
stop zone 1
set drmax 10
#
# other commands for details =========
#
# commands controlling output =========
normalize to "O  8" 18.9689A
save performance "grains_hot.per"
```

```
save overview "grains_hot.ovr" last
#
#
# grains_hot.in
# class limit
# ======================================
#
```

This tests the grains in an extreme condition - irradiation by an AGN near the illuminated face of the molecular torus. The gas is predominantly heated by the grain electron photo-ejection.

`grains_hot_wd01.in`

test temperature of gas and dust in high energy density environment

```
title test temperature of gas and dust in high energy density environment
#
# commands controlling continuum =========
table power law
energy density temp 550
#
# commands for density & abundances =========
hden 5.0
init "ism.ini"
abundances orion no grains
grains orion no qheat
#
# revert to WD01 treatment
no grain x-ray treatment
#
# commands controlling geometry =========
stop zone 1
set drmax 10
#
# other commands for details =========
#
# commands controlling output =========
normalize to "O 8" 18.9689A
save performance "grains_hot_wd01.per"
save overview "grains_hot_wd01.ovr" last
#
#
# grains_hot_wd01.in
# class limit
# ======================================
#
```

This tests the grains in an extreme condition - irradiation by an AGN near the illuminated face of the molecular torus. The gas is predominantly heated by the grains. The grain treatment has been reverted to Weingartner & Draine, 2001, which is NOT appropriate for these conditions. It is however a good test whether the old treatment is not broken....

`grains_lte.in`

check that grains equilibriate at correct temp in ste limit

```
title check that grains equilibriate at correct temp in ste limit
# this also tests that the code works when H He ionization is ZERO
#
# commands controlling continuum =========
black 3 lte
```

```
#
# commands for density & abundances =========
hden 5
eden 5
init file "hheonly.ini"
# need to normalize to some line, oxygen will provide some
element oxygen on
# ism grains with high dust to gas ratio
grain abund 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
cosmic rays background
database h2
#
# commands controlling output =========
save species "grains_lte.h" "H[:]" last densities
save species "grains_lte.h2" "H2[:]" last densities
normalize to "O 1" 63.1679m
save overview "grains_lte.ovr"
save performance "grains_lte.per"
save heating last "grains_lte.het"
save cooling last "grains_lte.col"
#
# grains_lte.in
# class limit
# ========================================
#
```

This test irradiates a set of grains with a true blackbody in strict thermodynamic equilibrium. We expect the grains (and everything else) to equilibriate at the blackbody temperature. The gas temperature is forced to the radiation temperature because the current molecule network (based on ISM approximations) does not go to LTE in the high-radiation density limit. The calculation asserts that all grain temperatures are very close to the radiation temperature.

`grains_qheat.in`

cool atomic ISM with Si grain quantum heating

```
title cool atomic ISM with Si grain quantum heating
#
# commands controlling continuum =========
table draine
extinguish 20
#
# commands for density & abundances =========
hden 0
# turns on grains with default abundance (log abundance ratio to ism = 0)
# and with quantum heating enabled by default
# (disabled with "no grains qheat" option)
grains 0. "silicate_ism_10.opc"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
cosmic rays background
iterate
#
# commands controlling output =========
normalize to "c 2" 157.636m
```

```
print line faint -2
print line column
save overview "grains_qheat.ovr"
save performance "grains_qheat.per"
save grains temperature last "grains_qheat.qht"
save continuum "grains_qheat.con" units microns last
save two photon continuum "grains_qheat.2nu" units microns
save qheat last "grains_qheat.qhd"
#
#
# grains_qheat.in
# class limit
# ======================================
#
```

This sim produces dust emission with a Wein trail that is dominated by quantum heating emission.

`grains_temp.in`

test all grain species temperature

```
title test all grain species temperature
#
# commands controlling continuum =========
black 50000
ionization parameter -2
#
# commands for density & abundances =========
hden 3
grains "graphite_ism_01.opc"
grains "silicate_ism_01.opc"
grains "graphite_orion_01.opc"
grains "silicate_orion_01.opc"
grains "silicate_0m010.opc"
grains "silicate_0m100.opc"
grains "grey_ism_01.opc"
grains "silicate_1m000.opc"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
iterate
constant temper 4
#
# commands controlling output =========
#
#
# grains_temp.in
# class limit
# ======================================
#
```

This turns on all the grain species that are included in the distribution. A model of an ionized layer is done and the monitors confirm the resulting grain temperatures.

`grains_temp_all.in`

test all grain species temperature

```
title test all grain species temperature
```

```
#
# commands controlling continuum =========
black 50000
ionization parameter -2
#
# commands for density & abundances =========
hden 3
# this turns on orion-style distributed grains
grains orion
# this turns on ism distributed grains
grains ism
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
constant temper 4
iterate
#
# commands controlling output =========
save overview "grains_temp_all.ovr"
save performance "grains_temp_all.per"
save dr "grains_temp_all.dr" last
save grain charge "grains_temp_all.grnchr" last
save grain temperature "grains_temp_all.grntem" last
save grain drift velocity "grains_temp_all.grndft" last
#
```

grains_temp_all.in # class limit # ==

This is a relatively quick test of grains. The Orion and ISM silicate and graphitic grains are turned on and their equilibrium temperature checked.

`grd_extreme_THiNhi.in`

slow/grid_extreme highest density highest temperature

```
title slow/grid_extreme highest density highest temperature
set save prefix "grd_extreme_THiNhi"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 6
#
hden 18
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grd_extreme_ThiNlo.in

slow/grid_extreme lowest density highest temperature

```
title slow/grid_extreme lowest density highest temperature
set save prefix "grd_extreme_ThiNlo"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 6
#
hden -8
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grd_extreme_TloNhi.in

slow/grid_extreme highest density lowest temperature

```
title slow/grid_extreme highest density lowest temperature
set save prefix "grd_extreme_TloNhi"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 1
#
hden 18
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

grd_extreme_TloNlo.in

slow/grid_extreme lowest density lowest temperature

```
title slow/grid_extreme lowest density lowest temperature
set save prefix "grd_extreme_TloNlo"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 1
#
hden -8
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grid_coronal.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
hden 0
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal.grd" last no hash
save ages "grid_coronal.age" last no hash
save cooling "grid_coronal.col" last no hash
#
# grid_coronal.in
# class coronal
# ======================================
```

```
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain the chemistry. This is a coronal (collisional) ionization calculation.

---

grid_coronal_grains.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
abundances ISM
grains PAH 3
hden 0
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal_grains.grd" last no hash
save cooling "grid_coronal_grains.col" last no hash
#
# grid_coronal_grains.in
# class coronal
# ======================================
#
*********
```

this is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation. This case uses ISM abundances, depleted heavy elements, with grains

---

grid_coronal_primal.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
hden 0
abundances primordial
#
# must include cosmic ray background since going below 1e4 K
# make it 1e-4 of the default rate
cosmic ray background -4
```

```
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal_primal.grd" last no hash
save cooling "grid_coronal_primal.col" last no hash
#
# grid_coronal_primal.in
# class coronal
# ======================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation.

This version uses primordial abundances. A small CR rate has to be set for the low-T chemistry to work. The possibility of primordial cosmic rays is rays is mentioned by 2014A&A...570L...3T although thiey are not part of standard primrodial chemistry networks.

This is not a realistic model for several reasons. First, it uses the approximate small H2 model - the large model invoked with ATOM H2 is better but slower. Second, primordial chemistry is time dependent - the Universe is typically not old enough, at a given z, for the chemistry to have reached steady state. This is a time-steady calculation.

The purpose of the test is to demonstrate code behavior in the metal-free limit, over a wide range of temperature. Gas-phase light-element chemistry is exercised, but with the trace amount of cosmic rays.

`grid_h2coronal.in`

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 log sequential
#
# commands for density & abundances =========
hden 0
# use all databases
database H2
database chianti levels max
database stout levels max
species "Fe+" levels=all
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_h2coronal.grd" last no hash
save cooling "grid_h2coronal.col" last no hash
#
# grid_h2coronal.in
# class coronal
# ======================================
```

```
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain the chemistry. This is a coronal (collisional) ionization calculation.

It is a pair with grid_coronal - this uses complete species models, including all levels, while grid_coronal uses the default. There will be more cooling as a result, at a cost of more memory and greater execution time. This also serves as a test of the full Stout database

---

grid_h2coronal_primal.in

coronal equilibrium

```
title coronal equilibrium
set save prefix "grid_h2coronal_primal"
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 log sequential
#
# commands for density & abundances =========
hden 0
abundances primrodial
database H2
#
# must include cosmic ray background since going below 1e4 K
# make it 1e-4 of the default rate
cosmic ray background -4
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid ".grd" last no hash
save cooling ".col" last no hash
#
# grid_h2coronal_primal.in
# class coronal
# ========================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation.

This version uses primordial abundances. A small CR rate has to be set for the low-T chemistry to work. The possibility of primordial cosmic rays is rays is mentioned by 2014A&A...570L...3T although thiey are not part of standard primrodial chemistry networks.

This is not a realistic model for several reasons. First, it uses the approximate small H2 model - the large model invoked with ATOM H2 is better but slower. Second, primordial chemistry is time dependent - the Universe is typically not old enough, at a given z, for the chemistry to have reached steady state. This is a time-steady calculation.

The purpose of the test is to demonstrate code behavior in the metal-free limit, over a wide range of temperature. Gas-phase light-element chemistry is exercised, but with the trace amount of cosmic rays.

---

h2_coll_t4.in

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 4
database H2
#
# commands controlling output =========
save performance "h2_coll_t4.per"
save overview "h2_coll_t4.ovr"
save continuum "h2_coll_t4.con" units angstroms
#
#
# h2_coll_t4.in
# class coronal
# ======================================
```

this tests conditions of collisional equilibrium at low densities

database h2 included to test results of large model Hden is 4 (coll_tx series is 10) to reproduce conditinos for major bug)

`h2_cr.in`

H2 with background cosmic ray ionization

```
title H2 with background cosmic ray ionization
#
# commands controlling continuum =========
# this is hot star SED
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate of 2.5e-17 s^-1,
cosmic rays, background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# failures should not occur
failures 1
database h2
iterate
# want clean test of CR physics so set constant kinetic temperature
constant temperature 500K
# must turn off line photoexcitation and Solomon process
```

```
# since we want to test cr heating and ionization
no induced processes
#
# commands controlling output =========
print column density
print ages
save performance "h2_cr.per"
save overview "h2_cr.ovr" last
save h2 lines "h2_cr.lin" last electronic all
save h2 rates "h2_cr.rat" last
save h2 column density "h2_cr.col" last
save dominant rates "h2_cr.h2" "H2" last
save chemistry rates "h2_cr.h2d" "H2" destruction
#
#
# h2_cr.in
# class limit
# ======================================
#
```

This test conditions of cosmic ray ionization. Solar abundances with no dust are assumed so this involves gas-phase chemistry alone. The Solomon process is disabled with the "no induced processes' command so H2 is mainly dissociated by cosmic rays. This forms a pair with h2_cr_grains, which does include grains.

`h2_cr_grains.in`

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
abundances ism
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
# must turn off line photoexcitation
# since we want to test cr heating and ionization
no induced processes
#
# commands controlling output =========
normalize to "H2 " 2.12125m
print column density
print ages
save performance "h2_cr_grains.per"
save overview "h2_cr_grains.ovr" last
save h2 lines "h2_cr_grains.lin" limit -10 last electronic all
```

```
save continuum units microns "h2_cr_grains.con" last
save h2 rates "h2_cr_grains.rat" last
save h2 column density "h2_cr_grains.col" last
save grains H2rates "h2_cr_grains.h2r" last
save dominant rates "h2_cr_grains.h2" "H2" last
save chemistry rates "h2_cr_grains.h2d" "H2" destruction
#
# h2_cr_grains.in
# class limit
# ======================================
#
```

This tests conditions of cosmic ray ionization and grain formation pumping. Solomon process is turned off with the "no induced processes" command so cosmic rays are the main dissociation process. This forms a pair with h2_cr which does not include grains, so relies only on gas-phase chemistry.

`h2_hminus.in`

H2 populations in H- dominated limit

```
title H2 populations in H- dominated limit
# this is one of a pair with h2_solomon.in
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
# no grains in this sim so H2 forms by H- route
abundances ism no grains
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# default is Takahashi 2001 - test thermal distribution here
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
#
# commands controlling output =========
print column density
print ages
save performance "h2_hminus.per"
save overview "h2_hminus.ovr" last
save h2 lines "h2_hminus.lin" last all
save h2 rates "h2_hminus.rat" last
save h2 column density "h2_hminus.col" last
save dominant rates "h2_hminus.h2" "H2" last
save chemistry rates "h2_hminus.h2d" "H2" destruction
#
# h2_hminus.in
# class limit
# ======================================
#
```

This tests large H2 model in limit of H- formation and Solomon destruction.

---

h2_pdr_leiden_f1.in

low density and flux model 1

```
title low density and flux model 1
set save prefix "h2_pdr_leiden_f1"
database H2 He collisions new
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
# this is to insure that no H-ionizing radiation strikes the cloud
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
# turn on the large H2 model
database h2
# turn down the number of convergence failures - there should be none
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the gas kinetic temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
# default normalization line is Hbeta, which is not produced by this gas
normalize to "c 2" 157.636m
print line faint -4
#
# saves
# check that all lines are found
table lines "LineList_PDR_H2.dat"
save performance ".per"
save overview ".ovr"
save fine optical depths last no hash ".fopt" range 1150 1300 units Angstroms 1
save save emitted continuum ".econ" range 1150 1300 units angstroms
save line emissivity ".ems"
H2 2.12125m
CO 650.074m
C 2 157.636m
O 1 63.1679m
Si 2 34.8046m
end of lines
save leiden lines ".lin"
save leiden ".lei"
save dr ".dr"
save molecules ".mol"
save grain physical conditions ".grn"
save overview ".ovr"
save H2 lines ".h2lin" all
save H2 column density ".h2col"
save H2 populations matrix zone ".pop"
save H2 rates ".rat"
```

```
save dominant rates ".h2" "H2"
save chemistry rates ".h2d" "H2" destruction
#
#
# h2_pdr_leiden_f1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

`h2_solomon.in`

H2 populations in solomon dominated limit

```
title H2 populations in solomon dominated limit
# this is a pair with h2_hminus
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
abundances ism
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# default is Takahashi 2001 - test thermal distribution here
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
#
# commands controlling output =========
# don't print so many lines
print line faint 10
print line column
print line sort wavelength
print column density
print ages
save performance "h2_solomon.per"
save overview "h2_solomon.ovr" last
save h2 lines "h2_solomon.lin" limit -10 last all electronic all
save h2 rates "h2_solomon.rat" last
save h2 column density "h2_solomon.col" last
save continuum units microns "h2_solomon.con" last
save dominant rates "h2_solomon.h2" "H2" last
save chemistry rates "h2_solomon.h2d" "H2" destruction
#
# h2_solomon.in
# class limit
# ======================================
#
```

This test H2 in case of grain formation and solomon destruction

---

h2_t2000.in

test large H2 molecule in shock-like conditions

```
title test large H2 molecule in shock-like conditions
#
# commands controlling continuum =========
# there is a continuum but it is unimportant
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
black 30000
intensity -5 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# must provide source of ionization for chemistry
cosmic rays, background
#
# commands for density & abundances =========
hden 6
grains ism, abundance log 0.16 single
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
#
# commands controlling geometry =========
stop zone 10
# force zone thickess to 1 cm
set dr 0
# need to lower stop temperature since gas is cooler than 4000K
stop temperature 3
#
# other commands for details =========
failures 2
database h2
constant temperature 2000
iterate
# this stop Lymnan line excitation of H, which is then photoionized
# by Balmer continuum
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "H2 " 2.12125m
#
save performance "h2_t2000.per"
save dominant rates "h2_t2000.oh" "OH" last
save dominant rates "h2_t2000.ohp" "OH+" last
save dominant rates "h2_t2000.h2" "H2" last
save pdr "h2_t2000.pdr"
save h2 rates "h2_t2000.rat"
save h2 column density "h2_t2000.col"
save h2 lines "h2_t2000.lin" all last
save h2 populations "h2_t2000.pop" all last
save chemistry rates "h2_t2000.h2d" "H2" destruction
save raw continuum "h2_t2000.raw"
save continuum "h2_t2000.con"
save overview "h2_t2000.ovr"
save species column densities "h2_t2000.scol" all
save species departures "h2_t2000.sdep" "H2O[:]"
save species densities "h2_t2000.spop" all
save species energies "h2_t2000.senr" "H2O[:]"
save species column densities "h2_t2000.scolH2O" "H2O[:]"
save species densities "h2_t2000.spopH2O" "H2O[:]"
#
# h2_t2000.in
```

```
# class limit
# ======================================
```

This is a collisionally dominated H2 simulation. The temperature has been fixed at 2000K and the large molecule turned on. The calculation checks the returned value of the ortho to para densities. Cosmic rays and the incident continuum have little effect, the density is high, so the populations should be close to LTE.

---

h2_t500.in

```
set h2 continuum dissociation Stancil
```

test large H2 molecule in PDR-like conditions

```
title test large H2 molecule in PDR-like conditions
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity -2.7 (total)
# this is hot star continuum
black 30000
intensity -5 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands for density & abundances =========
hden 6
grains ism, abundance log 0.16 single, no qheat
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
turbulence 2.7 km/sec
#
# commands controlling geometry =========
stop zone 10
# force zone thickess to 1 cm
sphere
set dr 0
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
#
# other commands for details =========
failures 2
database h2
constant temperature 500
iterate
Database H-like Lyman pumping off
cosmic rays background
#
# commands controlling output =========
normalize to "CO " 866.727m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print line faint -2
print ages
#
save performance "h2_t500.per"
save cooling "h2_t500.col"
save pdr "h2_t500.pdr"
save H2 rates "h2_t500.rat"
```

```
save H2 lines "h2_t500.lin" all
save H2 column density "h2_t500.h2col"
save H2 populations "h2_t500.pop"
save H2 levels "h2_t500.lev"
save raw continuum "h2_t500.raw"
save continuum "h2_t500.con"
save overview "h2_t500.ovr"
save dominant rates "h2_t500.h2" "H2"
save chemistry rates "h2_t500.h2d" "H2" destruction
#
# h2_t500.in
# class limit
# ======================================
```

This is a dense molecular gas with background cosmic rays and the incident radiation field set to a small value. The lower levels are in LTE.

---

h_otsopen.in

test ots, inward fractions for pure hydrogen, open geo, filling factor

```
title test ots, inward fractions for pure hydrogen, open geo, filling factor
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
constant temper 7500
filling factor 0.01
#
# other commands for details =========
# must iterate to get inward line fractions, that are asserted below
iterate
diffuse ots
# not iterating does not affect the solution
no level2
no induced processes (OK)
#
# commands controlling output =========
print line inward
save performance "h_otsopen.per"
save overview "h_otsopen.ovr" last
save dr "h_otsopen.dr" last
save continuum "h_otsopen.con" last units angstrom
#
# this is an open geometry, so do not expect H atom to exactly be case B
# due to Lyman line leakage. we iterated, so have a good estimate of
# inward and outward fractions, which we test
# h_otsopen.in
# class limit
# ======================================
#
```

This tests the total emission from a hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_otspp.in

plane parallel conservation and hydrogenic emission for pure hydrogen

```
title plane parallel conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
sphere static (OK)
#
# other commands for details =========
constant temper 7500
no level2
no induced processes (OK)
# needed to prevent 2s / Bal from becoming optically thick
turbulence 20 km/s
diffuse ots
database h-like levels resolved 10
#
# commands controlling output =========
save performance "h_otspp.per"
save overview "h_otspp.ovr"
save dr "h_otspp.dr"
#
# h_otspp.in
# class limit
# ======================================
#
```

This tests the total emission from a plane parallel pure hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

`h_otssp.in`

spherical conservation and hydrogenic emission for pure hydrogen

```
title spherical conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
radius 13
# not iterating does not affect the solution
sphere static (OK)
#
# other commands for details =========
constant temper 7500
diffuse ots
no level2
no induced processes (OK)
#
# commands controlling output =========
```

```
save performance "h_otssp.per"
save overview "h_otssp.ovr"
save dr "h_otssp.dr"
#
# h_otssp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_outopen.in

test open geometry

```
title test open geometry
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# commands controlling geometry =========
filling 0.01
#
# other commands for details =========
diffuse outward
iterate
database h-like levels resolved 15
no level2
no induced processes (OK)
constant temper 4
#
# commands controlling output =========
# normally will not print out inward parts of lines
print line inward
save performance "h_outopen.per"
save overview "h_outopen.ovr" last
save dr "h_outopen.dr" last
#
# this is an open geometry, so do not expect H atom to exactly be case B
# due to Lyman line leakage. we iterated, so have a good estimate of
# inward and outward fractions, which we test
# h_outopen.in
# class limit
# ======================================
#
```

This tests the total emission from an open geometry, hydrogen Stromgren sphere, using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_outpp.in

plane parallel H-only, close, test hydrogenic emission

```
title plane parallel H-only, close, test hydrogenic emission
#
```

```
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
# the hydrogen density
hden 5
# an ini file that will include H-only
init file "honly.ini"
#
# commands controlling geometry =========
# need this to prevent lyman lines from escaping
sphere static (OK)
#
# other commands for details =========
# prevent continuum pumping of lyman lines
no induced processes (OK)
# must include this to keep Ha optically thin
turbulence 20 km/s
# this is the approximation we are testing
diffuse outward
# force a constant temperature, then give stopping criteria
# if stop were not present model would go to limiting number of zones
constant temper 7500
# increase number of levels to get full emission
database h-like levels resolved 20
#
# commands controlling output =========
# need to turn this on so that continua at various energies will
# be included in the emission line list
# normalize results to perfect case b - our predictions should
# be close to this
# the output and asserts
save performance "h_outpp.per"
save overview "h_outpp.ovr"
save dr "h_outpp.dr"
#
# energies dominated by two photon emission not included since very
# sensitive to Lya transport
# h_outpp.in
# class limit
# ======================================
#
```

This tests the total emission from a plane parallel pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

`h_outsp.in`

spherical conservation and hydrogenic emission for pure hydrogen

```
title spherical conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
radius 13
# not iterating does not affect the solution
sphere static (OK)
```

```
#
# other commands for details =========
constant temper 7500
no level2
database h-like levels resolved 20
no induced processes (OK)
diffuse outward
#
# commands controlling output =========
save performance "h_outsp.per"
save overview "h_outsp.ovr"
save dr "h_outsp.dr"
#
# energies dominated by two photon emission not included since very
# sensitive to Lya transport
# h_outsp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_t4_conemis.in

continuous emission from H atom

```
title continuous emission from H atom
#
# commands controlling continuum =========
# use laser so that stellar continuum is not in predicted continuum
laser 2
ionization -1
#
# commands for density & abundances =========
# high density to suppress two-photon emission
hden 8
init "honly.ini"
#
# commands controlling geometry =========
# this thisckness is the inverse square of the density, so the
# total emission from the computed slab will in effect have the
# square of the density removed, so predictions will be j pi j / n_e n_p
stop thickness -16
#
# other commands for details =========
# include a large number of levels to capture IR emission
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
iterate
constant temperature 4
#
# commands controlling output =========
print lines column
save overview "h_t4_conemis.ovr"
save performance "h_t4_conemis.per"
save continuum "h_t4_conemis.con" last no title units microns
#
# h_t4_conemis.in
# class limit
# ======================================
#
```

This tests the continuous emission from the model H atom. The gas temperature is 10000 K and the continuous emissivity is asserted for a range of wavelengths.

This was used to generate the plot in Hazy 2 comparing the emission from a pure hydrogen plasma with those of Ferland 1980.

>>refer HI emission Ferland, G. J. 1980, PASP, 92, 596

---

h_t4_conemis_lon.in

low-den continuous HI emission with 2-nu important

```
title low-den continuous HI emission with 2-nu important
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 0
init "honly.ini"
#
# commands controlling geometry =========
stop thickness 0
#
# other commands for details =========
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
case b
iterate
constant temperature 4
#
# commands controlling output =========
print lines column
save overview "h_t4_conemis_lon.ovr"
save performance "h_t4_conemis_lon.per"
save continuum "h_t4_conemis_lon.con" last units microns
save two photon continuum "h_t4_conemis_lon.2nu" last rydbergs
#
# h_t4_conemis_lon.in
# class limit
# ======================================
#
```

This is a mate to hatomt10.in except that the density is low enough for two-photon emission to be very imporant in the optical and uv.

---

h_t4_conemis_thick.in

H I continuous emissivity, used for plot in hazy

```
title H I continuous emissivity, used for plot in hazy
#
# commands controlling continuum =========
black 5
ionization parameter -2
#
# commands for density & abundances =========
# high density to suppress two-photon emission
hden 7
# turn off all elements, except for hydrogen, so that
# we really test hydrogen emission
init file= "honly.ini"
```

```
#
# commands controlling geometry =========
# this is necessary to stop model at H ionization front
# constant temperature models will go on to infinity without this
stop efrac -0.8
#
# other commands for details =========
# increase continuum resolution by factor of ten
set continuum resolution 0.1
# line fluorescense would be very important with above turbulence,
# turn it off
no induced processes
# need large atom to get the many Rydgerg levels in the infrared
# atom h-like levels resolved 10
# what full outward flux so use spherical geometry
sphere
constant temperature 4
#
# commands controlling output =========
# results will be relative to interplated Hummer&Storey Hbeta
# this tests hydrogen atom too
# output the predicted continuum
save overview "h_t4_conemis_thick.ovr"
save performance "h_t4_conemis_thick.per"
save emitted continuum last iteration "h_t4_conemis_thick.con" units micron
save dr last "h_t4_conemis_thick.dr"
#
# h_t4_conemis_thick.in
# class limit
# ======================================
#
```

This checks that the predicted hydrogen continuum is in good agreement with exact results in the optically thin nebular limit.

Checks:
- This output was used to generate figure h_t4_conemis_thick in Part I of HAZY.
- Continuum relative to Hbeta should agree with Ferland (1980) filter averaged results.
- Hbeta should agree with Case B predictions, and Q(H) 4861.

`heatomt10.in`

continuous emission from HeI

```
title continuous emission from HeI
#
# commands controlling continuum =========
laser 1.9 ryd
ionization -1
#
# commands for density & abundances =========
# need high density to supress two-photon emission
hden 10
# force high density for electrons, He+ density will be the same
set eden 12
# set He/H ratio to 100, He and elec will have same density
element abundance helium 2
init "hheonly.ini"
#
# commands controlling geometry =========
# this thickness will get unit emission when combined with above densities
stop thickness -24
#
```

```
# other commands for details =========
iterate
constant temperature 4
#
# commands controlling output =========
#
set continuum resolution 0.1
set nFnu diffuse outward, diffuse inward
print line faint 1
print line column
save overview "heatomt10.ovr"
save performance "heatomt10.per"
save continuum "heatomt10.con" last no title units microns
save diffuse continuum "heatomt10.dif" last no title units microns
#
# heatomt10.in
# class limit
# ======================================
#
```

This tests continuous emission from the He I atom. The laser is used so that the incident continuum is not included in the total emission.

`heatomt10lon.in`

test low-den continuous emission from H atom, 2-nu is important

```
title test low-den continuous emission from H atom, 2-nu is important
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden -8
element helium abundance log 3
set eden -5
init "hheonly.ini"
#
# commands controlling geometry =========
stop thickness log 10
#
# other commands for details =========
no scattering opacity
# force all helium to be in He+
element helium ionization -4 0 -4
case b
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
iterate
constant temperature 4
#
# commands controlling output =========
normalize to "Blnd" 4472.76A vacuum
print lines column
print lines column
save overview "heatomt10lon.ovr"
save performance "heatomt10lon.per"
save continuum "heatomt10lon.con" last units microns
save diffuse continuum "heatomt10lon.dif" last units microns
save two photon continuum "heatomt10lon.2nu" last
#
# heatomt10lon.in
# class limit
```

```
# ======================================
#
```

This is a mate to hatomt10.in except that everything is He at low density

---

heiont10.in

continuous emission from HeII

```
title continuous emission from HeII
#
# commands controlling continuum =========
laser 5 ryd
ionization 1
#
# commands for density & abundances =========
hden 8
set eden 10
element abundance helium 2
init "hheonly.ini"
#
# commands controlling geometry =========
stop thickness -20
#
# other commands for details =========
constant temperature 4
iterate
# increase continuum resolution by factor of ten
set continuum resolution 0.1
set nFnu diffuse outward, diffuse inward
#
# commands controlling output =========
print line faint 1
print line column
save overview "heiont10.ovr"
save performance "heiont10.per"
save continuum "heiont10.con" last no title units microns
#
# heiont10.in
# class limit
# ======================================
#
```

This tests the He II continuous emission. The helium abundance is very large so that He II overwhelms other emission sources. The resolution of the continuum mesh is increased so that we get a better representation of the continuous emission.

---

helike_ar.in

He-like argon emission

```
title He-like argon emission
#
# commands controlling continuum =========
laser 600
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element argon abundance -2
```

```
element argon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element iron off
#
# commands controlling geometry =========
set dr -12
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure argon
print line faint -5
save overview "helike_ar.ovr"
save performance "helike_ar.per"
# This is Lyman alpha
normalize to "Ar17" 3.94907A
#
# 3.994A is 2^3S to ground
# Totl is 2^3P to ground
# 3.365A is 3^1P to ground
# 21.54A is 3^3P to 2^3S
# 22.24A is 3^3D to 2^3P
#
# helike_ar.in
# class limit
# ======================================
#
```

test He-like emission for argon

`helike_c.in`

he-like carbon emission

```
title he-like carbon emission
#
# commands controlling continuum =========
laser 50
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element carbon abundance -2
element carbon ionization -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element nitrogen off
element oxygen off
element neon off
```

```
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
set dr -12
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure carbon
print line faint -2
save overview "helike_c.ovr"
save performance "helike_c.per"
# This is Lyman alpha
normalize to "C 5" 40.2678A
#
#
# helike_c.in
# class limit
# ======================================
#
```

test he-like carbon emission

`helike_co.in`

He-like cobalt emission

```
title He-like cobalt emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure cobalt
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element cobalt on
# then set abundance and ionization after turning it on
element cobalt abundance -2
element cobalt ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
```

```
ionization -1
stop zone 1
print line faint -2
save overview "helike_co.ovr"
save performance "helike_co.per"
#
# helike_co.in
# class limit
# ======================================
#
```

test emission of He-like Co

`helike_cu.in`

He-like copper emission

```
title He-like copper emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure copper
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element copper on
# then set abundance and ionization after turning it on
element copper abundance -2
element copper ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 -5 -5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_cu.ovr"
save performance "helike_cu.per"
#
# helike_cu.in
# class limit
# ======================================
#
```

test emission of He-like Cu

`helike_fe.in`

he-like iron emission

```
title he-like iron emission
#
# commands controlling continuum =========
laser 1300
ionization -1
#
# commands for density & abundances =========
hden 7
set dr -12
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element iron abundance -2
element iron ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0
-5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print line faint -2
print he-like departure iron
save overview "helike_fe.ovr"
save performance "helike_fe.per"
# This is Lyman alpha
normalize to "Fe25" 1.8504A
#
#
# helike_fe.in
# class limit
# ======================================
#
```

check He-like emission for iron

`helike_mg.in`

he-like magnesium emission

```
title he-like magnesium emission
#
# commands controlling continuum =========
laser 250
ionization -1
#
# commands for density & abundances =========
hden 7
set dr -12
```

```
element magnesium abundance -2
element magnesium ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure magnesium
print line faint -2
save overview "helike_mg.ovr"
save performance "helike_mg.per"
# This is Lyman alpha
normalize to "Mg11" 9.16875A
#
#
# helike_mg.in
# class limit
# ======================================
#
```

test He-like Mg emission

`helike_n.in`

He-like nitrogen emission

```
title He-like nitrogen emission
#
# commands controlling continuum =========
laser 75
ionization -1
#
# commands for density & abundances =========
hden 7
element nitrogen abundance -2
element nitrogen ionization -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
```

```
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure nitrogen
print line faint -2
save overview "helike_n.ovr"
save performance "helike_n.per"
# This is Lyman alpha
normalize to "N 6" 28.7870A
#
# helike_n.in
# class limit
# ======================================
#
```

test He-like emission for N

`helike_ne.in`

he-like neon emission

```
title he-like neon emission
#
# commands controlling continuum =========
laser 170
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element neon abundance -2
element neon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure neon
```

```
print line faint -2
save overview "helike_ne.ovr"
save performance "helike_ne.per"
# This is Lyman alpha
normalize to "Ne 9" 13.4471A
#
#
# helike_ne.in
# class limit
# ======================================
#
```

test He-like emission for oxygen

`helike_ni.in`

he-like nickel emission

```
title he-like nickel emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure nickel
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element nickel on
# then set abundance and ionization after turning it on
element nickel abundance -2
element nickel ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 -5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_ni.ovr"
save performance "helike_ni.per"
#
# helike_ni.in
# class limit
# ======================================
#
```

Test He-like Ni emission.

`helike_o.in`

he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3

```
title he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
#
# commands controlling continuum =========
laser 100
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element oxygen abundance -2
element oxygen ionization -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure oxygen
print line sort wavelength
print line faint -5
save overview "helike_o.ovr"
save performance "helike_o.per"
save continuum "helike_o.con" units Angstroms
normalize to "o 7" 21.6020A
#
# helike_o.in
# class limit
# ======================================
#
```

test He-like emission for oxygen

---

helike_si.in

He-like silicon emission

```
title He-like silicon emission
#
# commands controlling continuum =========
laser 350
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
```

```
element silicon abundance -2
element silicon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure silicon
print line faint -2
save overview "helike_si.ovr"
save performance "helike_si.per"
# This is Lyman alpha
normalize to "Si13" 6.64803A
#
#
# helike_si.in
# class limit
#
```

test He-like emission for silicon

`helike_zn.in`

He-like zinc emission

```
title He-like zinc emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure zinc
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element zinc on
# then set abundance and ionization after turning it on
element zinc abundance -2
element zinc ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 
```

```
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_zn.ovr"
save performance "helike_zn.per"
#
# helike_zn.in
# class limit
# ======================================
#
```

test emission for He-like Zn

---

hhe_otspp.in

plane parallel conservation and H-like emission for H, He

```
title plane parallel conservation and H-like emission for H, He
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
# expanding sphere to stop Lya from destroying HeI 23S
sphere
#
# other commands for details =========
diffuse ots
database h-like element hydrogen levels resolved 10
# need to iterate since we will assert helium triplet lines
# that depend on having stable solution
iterate
constant temper 7500
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_otspp.per"
save overview "hhe_otspp.ovr" last
save dr "hhe_otspp.dr" last
#
# helium lines
# hhe_otspp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure H + He Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

hhe_otssp.in

spherical conservation and H-like emission for H and He

```
title spherical conservation and H-like emission for H and He
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
diffuse ots
database h-like levels resolved 10
radius 13
sphere static
#
# other commands for details =========
constant temper 7500
iterate
no level2
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_otssp.per"
save overview "hhe_otssp.ovr" last
save dr "hhe_otssp.dr" last
#
# helium lines
# hhe_otssp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure H + He-like Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked. The geometry is plane paralel.

`hhe_outpp.in`

plane parallel conservation emission for H, He gas

```
title plane parallel conservation emission for H, He gas
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
# open sphere to stop Lya from destroying HeI 23S
sphere
#
# other commands for details =========
# need this since will assert helium triplet lines that depend on stable soln
iterate
constant temper 7500
database h-like element hydrogen levels resolved 10
no level2
```

```
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_outpp.per"
save overview "hhe_outpp.ovr" last
save dr "hhe_outpp.dr" last
#
# hhe_outpp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

`hhe_outppff.in`

plane parallel filling factor pure H, He gas

```
title plane parallel filling factor pure H, He gas
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
filling factor -1
sphere
#
# other commands for details =========
# need this since will assert helium triplet lines that depend on stable soln
iterate
constant temper 7500
no level2
no induced processes (OK)
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
save performance "hhe_outppff.per"
save overview "hhe_outppff.ovr" last
save dr "hhe_outppff.dr" last
#
# helium lines
# hhe_outppff.in
# class limit
# ======================================
#
```

This is a plane-parallel constant temperature cloud with only hydrogen and helium. The gas has a filling factor of 0.1. Induced processes are turned off and a large H atom is used so that the hydrogen recombination spectrum will be close to Case B. The calculation stops beyond the hydrogen ionization front, because of the stop efrac command (it needs this since this is a constant temperature calculation, so the usual lower-temperature stopping criterion does not apply). The asserts confirm that energy is conserved and that the hydrogen spectrum is correct.

`hhe_outsp.in`

spherical conservation and H-like emission for H, He

```
title spherical conservation and H-like emission for H, He
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
radius 13
sphere static
#
# other commands for details =========
iterate
diffuse outward only
constant temper 7500
no level2
no induced processes (OK)
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
save performance "hhe_outsp.per"
save overview "hhe_outsp.ovr" last
save dr "hhe_outsp.dr" last
#
# helium lines
#
# hhe_outsp.in
# class limit
# ========================================
#
```

This tests a spherical cloud with only hydrogen and helium. Diffuse fields are transferred with the outward only approximation. The asserts check that the ionizing radiation is conserved.

`hii_blister.in`

Lexington 1995 dust-free hii blister region

```
title Lexington 1995 dust-free hii blister region
#
# commands controlling continuum =========
# a simple blackbody
blackbody 40000
# the flux of H-ionizing photons
phi(h) 13.0
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden 4
init file="ism.ini"
# HII region abundance but no dust
abundances hii region no grains
abundances he=1 c=1 n=1 o=1 ne=1 mg=.0001 si=.01 s=1 cl=1 ar=1
continue fe=.001
#
# commands controlling geometry =========
sphere
#
# other commands for details =========
# this is to desaturate Lya to prevent excited state photoionization
```

```
# from being important - the other codes did not include this important
# physical process
turbulence 10 km/s
# must iterate since optically thick
iterate
#
# commands controlling output =========
normalize to "Ca B" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line faint .01
print line sum
Blnd 5875.66A
blnd 2326
blnd 1335
blnd 1909
N 2 6583.45
N 2 6548.05
n 3 57.3238m
blnd 7325
blnd 3727
O 3 51.8004m
o 3 5006.84
o 3 4958.91
Ne 2 12.8101m
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
S 3 18.7078m
S 3 9530.62
S 3 9068.62
s 4 10.5076m
end of lines
set blend "HepsNe3" 3968
Ne 3 3967.47
H 1 3970.07
end of lines
save performance "hii_blister.per"
save overview last "hii_blister.ovr"
save dr last "hii_blister.dr"
save results last "hii_blister.rlt"
print line optical depths
#
#
# hii_blister.in
# class hii
# ======================================
```

This is one of the test cases from the Lexington Meeting suite of nebulae (Ferland et al. 1995). It is a grain-free hii_blister HII region, similar to inner regions of the Orion Nebula, except for the absence of grains. The set of lines entered with the print line sum command lists the most powerful coolants in this model. This is one of the tabulated quantities in the Lexington Meeting, and is a fundamental test of energy conservation in the code. The ratio of the sum of these lines to Hb is equivalent to the Stoy ratio, used for determining stellar temperatures.

The "dielec kludge 0" command is to turn off my estimates of the DR rates for those elements that had none. This was only to allow comparison with other calculations that did not make similar estimates. For an actual calculation I would not include this command, since the guesses are better than nothing.

the turbulence is to stop the balmer lines from becoming optically thick since few other codes include an actual H atom, but use case b instead. The Orion HII region does have an observed turbulence of about 8 km/s.

This calculation stops near the H+ - H0 ionization front, where the temperature falls below the default lowest temperature of 4000 K. This model would have continued into the PDR had a lower temperature been specified with the STOP LOWEST TEMP command.

---

hii_coolstar.in

dust free cool HII region model, Lexington 1995

```
title dust free cool HII region model, Lexington 1995
#
# commands controlling continuum =========
black body, T = 20000 K
q(h) 49
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden = 2
init file="ism.ini"
abund He=-1 C=-3.6576 N=-4.39794 O=-3.481146 ne=-4.30103 mg=-8
continue si=-8 s=-5.04576 cl=-7 ar=-8 fe=-8
#
# commands controlling geometry =========
radius = 18.477121
sphere
# this is to go deep to pick up all H recombs
stop efract -2
stop temperature 1000
#
# other commands for details =========
# must iterate since fine structure lines are optically thick
iterate
# assume there is neutral gas beyond what we compute
double
#
# commands controlling output =========
print line faint .01
# this is the sum of lines in table 2 of the Lexington meeting
print line sum
N 2 6583.45
N 2 6548.05
blnd 3727
Ne 2 12.8101m
Blnd 6720
S 3 18.7078m
S 3 33.4704m
S 3 9530.62
S 3 9068.62
end of lines
save performance "hii_coolstar.per"
save overview last "hii_coolstar.ovr"
save dr last "hii_coolstar.dr"
save results last "hii_coolstar.rlt"
save continuum last units microns "hii_coolstar.con"
save lines, zone cumulative, "hii_coolstar.cum"
H 1 4861.32A
o 3 5006.84
blnd 3727
O 1 6300.30
end of lines
#
# Hbeta 4.93E36, L(total)4.30xHbeta
# hii_coolstar.in
# class hii
# ======================================
#
```

This is one of the test cases from the Lexington Meeting suite of nebulae. It is a grain-free HII region ionized by a very cool star. Hydrogen is ionized but not helium so this tests the transport of the H Lyman continuum. The set of lines is entered with the print line sum command to test energy conservation.

hii_hiU_StaticSphere_noGrains.in

very high ionization parameter static H II region without dust

```
title very high ionization parameter static H II region without dust
stop efrac -1
stop temperature 3
sphere static
covering factor 0.500
q(H) = 51.340
radius 1.000 linear parsecs
hden 2.
database h-like element hydrogen resolved levels 20
print line pump
iterate to convergence
```

test

```
title test
# IMF slope: 2.35 Mup=120 Mlow=0.1 Mo
# Metallicity: z004 ;
# Age = 2.9000 Myrs
print off
interpolate ( 6.5172, -10.0000)
continue (12.2727001 , 18.5331989 ) (12.3306917 , 18.4600873 )
continue (12.3976394 , 18.3696100 ) (12.4768200 , 18.2559724 )
continue (12.5737312 , 18.1106805 ) (12.6986694 , 17.9237063 )
continue (12.8747606 , 17.7132364 ) (13.1757900 , 17.9262936 )
continue (13.4759529 , 18.4762233 ) (13.4776898 , 18.4795692 )
continue (13.4794342 , 18.4830526 ) (13.4811860 , 18.4865412 )
continue (13.4829436 , 18.4900359 ) (13.4847097 , 18.4935365 )
continue (13.4864815 , 18.4970429 ) (13.4882616 , 18.5005546 )
continue (13.4900484 , 18.5040724 ) (13.4918434 , 18.5075965 )
continue (13.4936462 , 18.5111264 ) (13.4954555 , 18.5146620 )
continue (13.4972725 , 18.5182046 ) (13.4990971 , 18.5217529 )
continue (13.5009291 , 18.5253099 ) (13.5027698 , 18.5288689 )
continue (13.5046176 , 18.5324342 ) (13.5064739 , 18.5360110 )
continue (13.5083371 , 18.5395916 ) (13.5102098 , 18.5431760 )
continue (13.5120904 , 18.5467681 ) (13.5139776 , 18.5503718 )
continue (13.5158738 , 18.5539755 ) (13.5177790 , 18.5569388 )
continue (13.5196928 , 18.5608904 ) (13.5216140 , 18.5648526 )
continue (13.5235449 , 18.5688178 ) (13.5254828 , 18.5727940 )
continue (13.5274301 , 18.5767735 ) (13.5293867 , 18.5807617 )
continue (13.5313524 , 18.5847603 ) (13.5333258 , 18.5887622 )
continue (13.5353093 , 18.5927732 ) (13.5373014 , 18.5967928 )
continue (13.5393032 , 18.6008181 ) (13.5413133 , 18.6048488 )
continue (13.5433328 , 18.6088943 ) (13.5453628 , 18.6129424 )
continue (13.5474018 , 18.6169987 ) (13.5494508 , 18.6210632 )
continue (13.5515086 , 18.6251325 ) (13.5535772 , 18.6292082 )
continue (13.5556542 , 18.6332996 ) (13.5577429 , 18.6373981 )
continue (13.5598408 , 18.6415044 ) (13.5619489 , 18.6456182 )
continue (13.5640669 , 18.6497377 ) (13.5661958 , 18.6538678 )
continue (13.5683355 , 18.6580066 ) (13.5704857 , 18.6621496 )
continue (13.5726463 , 18.6663076 ) (13.5748181 , 18.6704725 )
continue (13.5769998 , 18.6746433 ) (13.5791935 , 18.6788257 )
continue (13.5813978 , 18.6830186 ) (13.5836136 , 18.6872189 )
continue (13.5858407 , 18.6914292 ) (13.5880800 , 18.6956417 )
continue (13.5903301 , 18.6998759 ) (13.5925920 , 18.7041127 )
continue (13.5948653 , 18.7083589 ) (13.5971520 , 18.7126123 )
continue (13.5994497 , 18.7168416 ) (13.6017591 , 18.7167174 )
continue (13.6040823 , 18.7210062 ) (13.6064168 , 18.7296665 )
continue (13.6087645 , 18.7334982 ) (13.6111251 , 18.7383992 )
continue (13.6134983 , 18.7433132 ) (13.6158838 , 18.7482317 )
```

```
continue (13.6182835 , 18.7531594 ) (13.6206960 , 18.7581142 )
continue (13.6231221 , 18.7630629 ) (13.6255625 , 18.7680391 )
continue (13.6280158 , 18.7730141 ) (13.6304838 , 18.7780038 )
continue (13.6329652 , 18.7830126 ) (13.6354616 , 18.7880218 )
continue (13.6379718 , 18.7930573 ) (13.6404963 , 18.7980966 )
continue (13.6430359 , 18.8031500 ) (13.6455912 , 18.8082162 )
continue (13.6481609 , 18.8132926 ) (13.6507455 , 18.8183811 )
continue (13.6533466 , 18.8234835 ) (13.6559630 , 18.8285902 )
continue (13.6585952 , 18.8337279 ) (13.6612427 , 18.8388661 )
continue (13.6639072 , 18.8440242 ) (13.6665882 , 18.8491877 )
continue (13.6692853 , 18.8543793 ) (13.6713201 , 18.8582681 )
continue (13.6726815 , 18.8608745 ) (13.6740469 , 18.8634738 )
continue (13.6754172 , 18.8660834 ) (13.6767914 , 18.8686938 )
continue (13.6781704 , 18.8713110 ) (13.6795533 , 18.8739280 )
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continue (16.4446053 , 9.9753257 ) (16.4531562 , 9.7229785 )
continue (16.4606228 , 9.5066902 ) (16.4682203 , 9.2903934 )
continue (16.4785607 , 8.9416311 ) (16.4869261 , 8.4270799 )
continue (16.4940975 , 7.9941810 ) (16.5060096 , 7.2913992 )
continue (16.5182572 , 6.5892987 )continue ( 22.38, -10.0000)
print on
#
save performance "hii_hiU_StaticSphere_noGrains.per"
save overview "hii_hiU_StaticSphere_noGrains.ovr"
save dr "hii_hiU_StaticSphere_noGrains.dr"
#
#
#
#
#
#
#
# H II region
```

This model was added to have at least one sim with a very high ionization parameter and a grain-free static closed geometry to maximize line trapping.

`hii_icf.in`

HII region with negative He/H ICF

```
title HII region with negative He/H ICF
#
# commands controlling continuum =========
# this is the result of this command
# table star mihalas 46000
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_mihalas_46000.dat"
ionization parameter -2.
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden 3
init file "ism.ini"
abundances ism no grains
grains no qheat single
metals and grains 0.320
#
# commands controlling geometry =========
stop efrac -3
stop temperature 15
sphere
#
# other commands for details =========
failures 1
#
# commands controlling output =========
save performance "hii_icf.per"
save overview "hii_icf.ovr" last
save dr "hii_icf.dr" last
#
```

```
# hii_icf.in
# class hii
# ======================================
```

This is an example of an H II region irradiated by a hard stellar continuum - one of the Mihalas NLTE stars. The hard continuum produces a negative He/H ionization correction factor, as discussed in Ballantyne, Ferland & Martin (2000). >>refer HeI icf by Ballantyne,D.R., Ferland, G.J., & Martin, P.G., 2000, ApJ 536, 773-777

---

hii_paris.in

"New" Paris meeting HII region

```
title "New" Paris meeting HII region
# "standard" HII region model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 40000 K radius = 12.113943
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden = 2
init file="ism.ini"
element aluminium on
element helium abundance -1
element carbon abundance -3.6576
element nitrogen abundance -4.39794
element oxygen abundance -3.481146
element neon abundance -4.30103
element magnesium abundance -8
element aluminium abundance -8
element silicon abundance -8
element sulphur abundance -5.04576
element chlorine abundance -7
element argon abundance -8
element iron abundance -8
#
# commands controlling geometry =========
radius = 18.477121
sphere
# next two to make sure we pick up all possible H recombination
set temperature floor 1000
# make sure sim goes very deep into cold gas
stop temperature 100K
stop efrac -2
#
# other commands for details =========
# must iterate since fine structure lines are optically thick
iterate
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
normalize to "Ca B" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print column densities
print line optical depths
print line faint 0.01
print line sum
Blnd 5875.66A
blnd 2326
blnd 1909
n 2 121.769m
N 2 6583.45
N 2 6548.05
```

```
n 3 57.3238m
blnd 3727
o 3 5006.84
o 3 4958.91
O 3 51.8004m
O 3 88.3323m
Ne 2 12.8101m
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
Blnd 6720
S 3 18.7078m
S 3 33.4704m
S 3 9530.62A
S 3 9068.62
s 4 10.5076m
end of lines
save performance "hii_paris.per"
save overview last "hii_paris.ovr"
save each cooling last "hii_paris.cole"
save cooling last "hii_paris.col"
save hydrogen 21 cm last "hii_paris.21cm"
save results last "hii_paris.rlt"
save dr last "hii_paris.dr"
save linelist "hii_paris.lin" "LineList_HII.dat" last no hash column
# this is to confirm that this commnand works
save lines emissivity "hii_paris.str" last
H 1 4861.32A
end lines
#
table lines "LineList_HII.dat"
# hii_paris.in
# class hii
# ======================================
#
```

This is one of the "standard" models computed at the Paris and Lexington meetings on photoionization and shock calculations. a bable in hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes. It is necessary to iterate since some fine structure lines are optically thick. The set of lines entered with the print line sum command is used to obtain the total luminosity in detected lines, a measure of the Stoy temperature.

Checks:
- Hb close to case B, Q(H) 4861, intensities.
- Enter answers in Table Error! Reference source not found..

`hii_Um3.in`

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um3"
Blackbody 56000
ionization parameter = -3.000
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
#
save last continuum ".con" units microns
save last overview ".ovr"
```

```
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hii_Um35.in

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um35"
Blackbody 56000
ionization parameter = -3.5
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
#
save last continuum ".con" units microns
save last overview ".ovr"
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hii_Um385.in

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um385"
Blackbody 56000
ionization parameter = -3.85
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
#
save last continuum ".con" units microns
save last overview ".ovr"
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hlike_c.in

H-like C VI case B

```
title H-like C VI case B
#
# commands controlling continuum =========
table agn
ionization parameter 3
#
# commands for density & abundances =========
hden = 8
init file="ism.ini"
element carbon abundance 1
set eden 9
#
# commands controlling geometry =========
set dr -18
stop zone 1
#
# other commands for details =========
case b hummer no photoionization
no induced processes (OK)
constant temperature = 1.e5
#
# commands controlling output =========
save overview "hlike_c.ovr"
save performance "hlike_c.per"
save results "hlike_c.rlt"
#
# hlike_c.in
# class limit
# ======================================
#

This test case compares the predictions of the multi-level H-like CVI atom
with the Storey and Hummer (1995) results. The set dr command sets the
zone thickness to 1 cm. The case b command sets Lyman line optical depths
to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities
```

---

hlike_o.in

H-like O VIII case B

```
title H-like O VIII case B
#
# commands controlling continuum =========
table agn
ionization parameter 4
#
# commands for density & abundances =========
hden = 8
init file="ism.ini"
element oxygen abundance 1
set eden 9
#
# commands controlling geometry =========
# set following so the n^2 dr is unity
set dr -18
```

```
stop zone 1
#
# other commands for details =========
case b hummer no photoionization
no induced processes (OK)
constant temperature = 1.e5
# Resolve O 8 Lya doublet
database h-like lyman extra resolution 0.01
database h-like oxygen resolved levels 10
database h-like oxygen collapsed levels 10
#
# commands controlling output =========
print lines sort wavelength
print lines column
save overview "hlike_o.ovr"
save performance "hlike_o.per"
save results "hlike_o.rlt"
#
# hlike_o.in
# class limit
# ======================================
#

This test case compares the predictions of the multi-level H-like O VIII atom
with the Storey and Hummer (1995) results. The set dr command sets the
zone thickness to 1 cm. The case b command sets Lyman line optical depths
to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities
```

---

igm_lalpha.in

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm05 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop "H" column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
set save prefix "igm_lalpha"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# on 05 aug 29 changed from old background command to
# cmb 2 plus hm05 z=2 background - all results changed substantially
# igm_lalpha.in
# class igm
# ======================================
#
```

```
This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim corrects line intensities for isotropic continua. Its sister sim, igm_lalpha_noisosub.in, computes intensities uncorrected for isotropic continua.

`igm_lalpha_hm12.in`

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm12 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
set save prefix "igm_lalpha_hm12"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# igm_lalpha_hm12.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim corrects line intensities for isotropic continua. Its sister sim, igm_lalpha_noisosub_hm12.in, computes intensities uncorrected for isotropic continua.

`igm_lalpha_noisosub.in`

Ly alpha forest cloud

```
title Ly alpha forest cloud
```

```
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm05 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
no lines isotropic continuum subtraction
set save prefix "igm_lalpha_noisosub"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# on 05 aug 29 changed from old background command to
# cmb 2 plus hm05 z=2 background - all results changed substantially
# igm_lalpha_noisosub.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim computes line intensities not corrected for isotropic continua (see the "no lines..." command above). Its sister sim, igm_lalpha.in, computes intensities corrected for isotropic continua.

`igm_lalpha_noisosub_hm12.in`

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm12 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
no lines isotropic continuum subtraction
```

```
set save prefix "igm_lalpha_noisosub_hm12"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# igm_lalpha_noisosub_hm12.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim computes line intensities not corrected for isotropic continua (see the "no lines..." command above). Its sister sim, igm_lalpha_hm12.in, computes intensities corrected for isotropic continua.

`igm_perseus.in`

Perseus cluster

```
title Perseus cluster
# model of IGM in Perseus galaxy cluster inspired by Hitommi spectroscopy
set save prefix "igm_perseus"
#
# assume gas is in collisional equilibrium
coronal 4.6e7K
#
# commands for density & abundances =========
hden -1.5
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# adjust models to get higher accuracy
database H-like element iron resolved levels 10
database H-like element iron collapsed levels 50
database He-like element iron resolved levels 10
database He-like element iron collapsed levels 50
iterate to convergence
#
# commands controlling output =========
print line column
print line sort wavelength
print line faint -2
print line faint off
#print line sort intensity
normalize "Fe25" 1.85040A 1
save overview ".ovr"
save performance ".per"
save element oxygen ionization ".oxy"
save element iron ionization ".fe"
save performance ".per"
#
#
#
#
#
#
```

```
#
#
#
#
#
#
#
#
****************************
# agn_erseus.in, hot gas in the Perseus galaxy cluster
# class igm
# ================================
#
```

This is inspired by Hitomi observations of the Fe complex in Perseus and has been developed by Priyanka Chakraborty as part of her thesis.

`igm_primal.in`

cloud with primordial abundances exposed to background at Z=10

```
title cloud with primordial abundances exposed to background at Z=10
#
# commands controlling continuum =========
background, redshift= 10
# background due to agn from Haardt & Madau 1996 ApJ, 461, 20
# this sets both continuum shape and intensity, actually for z=2
table HM96 old
#
# other commands for details =========
# put in a velocity field to stop Lya from causing stability problems
turbulence 20 km/s
# do a second iteration to establish that it is optically thick downstream
iterate
# this sim should run cleanly - do not accept problems
failures 2
#
# commands for density & abundances =========
# this log of the hydrogen density
hden 5
# stored set of primordial abundances
abundances primordial
#
# commands controlling geometry =========
# we want to shielded face to not be exposed to empty space, but rather
# be just very deep in a dense cloud - this prevents lines from freely
# radiating from the shielded face
double optical depths
# set a lower temperature stopping criterion - default is 4000K
stop temperature 30
#
# commands controlling output =========
# don't want to print lots of faint hydrogen lines
print line faint -3
# some output files with info we want to save
save performance "igm_primal.per"
save temperature history "igm_primal_tem.his"
save ionizing continuum "igm_primal.ion"
save hydrogen conditions "igm_primal.mol"
save heating "igm_primal.het"
save dr "igm_primal.dr"
save cooling "igm_primal.col"
save overview "igm_primal.ovr"
save results last "igm_primal.rlt"
#
```

```
# igm_primal.in
# class hii pdr igm
# ======================================

This is a high redshift cloud irradiated by the cosmic background and AGN light.
H- absorption of the z=10 cosmic background is a MAJOR heating agent
This model is very sensitive to treatment of Lya destruction, since resulting
J-bar is major destruction process for H-, which is the H2 formation route.
Lya ots oscillations could develop and are damped by not reevaluating H-
photo rate after first n times, as in hmole.c
```

---

igm_z3.in

redshift 1000 recombination epoch

```
title redshift 1000 recombination epoch
#
# commands controlling continuum =========
# a true blackbody radiation field, in strict thermodynamic equilibrium
blackbody 3000 STE
#
# commands for density & abundances =========
hden 0
abundances primordial
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
case b
iterate
#
# commands controlling output =========
normalize lines to "Ca B" 4861.32A
print ages
print departure coef element hydrogen
print line faint -5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "igm_z3.ovr"
save performance "igm_z3.per"
save dr "igm_z3.dr"
#
# igm_z3.in
# class limit igm
# ======================================
#
```

This is a model of the universe near the recombination epoch, at a redshift of a thousand. The gas is exposed to a true blackbody at 3000 K, and the abundances are primordial.

---

igm_z3_thick.in

redshift 1000 recombination epoch

```
title redshift 1000 recombination epoch
#
# commands controlling continuum =========
# A true blackbody radiation field, in strict thermodynamic equilibrium.
# This is a resolved variant of igm_z3, which should have uniform conditions.
blackbody 3000 STE
```

```
#
# commands for density & abundances =========
hden 0
abundances primordial
#
# commands controlling geometry =========
# stop zone 1
stop thickness 16
stop temperature 0
#
# other commands for details =========
case b
iterate
#
# commands controlling output =========
normalize lines to "Ca B" 4861.32A
print ages
print departure coef element hydrogen
print line faint -5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "igm_z3_thick.ovr"
save performance "igm_z3_thick.per"
save dr "igm_z3_thick.dr"
#
# igm_z3_thick.in
# class limit igm
# ======================================
#
```

This is a model of the universe near the recombination epoch, at a redshift of a thousand. The gas is exposed to a true blackbody at 3000 K, and the abundances are primordial.

This is a spatially-resolved variant of igm_z3, which should have uniform conditions throughout the depth.

`ism.in`

cloud irradiated by ism background

```
title cloud irradiated by ism background
#
# commands controlling continuum =========
# this uses the Black continuum with no H-ionizing radiation,
# and with background cosmic rays
cmb
table ism
extinguish by a column of 22
# need cosmic rays to provide ionization to the chemistry
cosmic rays, background
#
# commands for density & abundances =========
hden 0
init file="ism.ini"
abundances ism
#
# commands controlling geometry =========
# set sphere since matter in all directions
sphere
stop temperature linear 10
stop thickness 0.1 linear parsecs
#
# other commands for details =========
# this prevents continuum pumping from exciting H0
Database H-like Lyman pumping off
# this is to converge optical depths
```

```
iterate
# this should have no effect since T is larger than 100 K
set temperature floor 100K
#
# commands controlling output =========
# this model has no heavy element molecules, because H2 does not
# really fully form, since Lyman bands are not self-shielded
normalize to "C 2" 157.636m
print line pump
save performance "ism.per"
save overview "ism.ovr" last
save dr "ism.dr"
save heating "ism.het"
save coolign "ism.col"
save continuum "ism.con" units microns last
save continuum "ism.con-no-iso" units microns last no isotropic
#
# ism.in
# class ism
# ======================================
```

TODO - look at temperature struture - it has jitter at about the level of convergence, up and down. Temp jitter caused by eden jitter. This model is nearly isothermal, jitter measures noise in solver, and is great chance to pin this down.

This is a test of the behavior of the code in the extreme of photoionization by a relatively hard continuum, at low densities. The continuum is the galactic background, attenuated by a column density of 10^22 cm-2. Ionization by galactic background cosmic rays is included. Database H-like Lyman pumping off appears since this region is deep in the ISM, and the Lyman lines are quite thick. This example checks whether the ionization balance, thermal balance, and electron density sum, are performed correctly in this limit.

Checks:
- Numerical stability of solution
- Thickness exact

`ism_cosmicray.in`

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
# background CR H0 ionization rate should be 2.5e-17 s^-1,
# Williams et al. ApJ, 503, 689
cosmic rays, background
# this will be VERY faint black 50000
ionization parameter -25
black 50000
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
set temperature floor 1000 K
# turn off molecules to test only ions
no molecules
# must turn off charge transfer and its heating, which would dominate,
# since we want to test cr heating and ionization
```

```
no charge transfer
no ctheat
# must turn of photoionization by recombining species,
# since we want to test cr heating and ionization
no photoionization
# any time photoionization is turned off, it is best to also
# turn off induced processes, which include pumping in the lyman lines
no induced processes
#
# commands controlling output =========
print ages
save overview "ism_cosmicray.ovr"
save performance "ism_cosmicray.per"
#
# ism_cosmicray.in
# class limit
# ========================================
#
```

This test conditions of cosmic ray ionization. Molecules and charge transfer are disabled so that analytical estimates can be made.

`ism_grid.in`

interstellar cloud irradiated by ism background

```
title interstellar cloud irradiated by ism background
#
# commands controlling continuum =========
# this uses the Black continuum with no H-ionizing radiation,
# and with background cosmic rays
table ism
extinguish by a column of 22
cosmic rays background linear 0.1266
#
# commands for density & abundances =========
hden 0 vary
grid from -3 to 2 in 0.5 dex steps sequential
init file="ism.ini"
# this turns on ism abundances and grains
abundances ism
#
# commands controlling geometry =========
# set sphere since matter in all directions
sphere
stop temperature linear 10
stop thickness 0.1 linear parsecs
stop zone 1
#
# other commands for details =========
# this prevents continuum pumping from exciting H0
Database H-like Lyman pumping off
#
# commands controlling output =========
# this model has no heavy element molecules, because H2 does not
# really fully form, since Lyman bands are not self-shielded
normalize to "C 2" 157.636m
save performance "ism_grid.per"
save pressure "ism_grid.pre" last no hash
save grid "ism_grid.grd" last no hash
save averages "ism_grid.avr" last no hash
temperature hydrogen 1
end of averages
save overview "ism_grid.ovr" last
save dr "ism_grid.dr"
```

```
save heating "ism_grid.het" last no hash
save coolign "ism_grid.col" last no hash
save xspec mtable "ism_grid.fit" range 0.1 3 keV
save temperature "ism_grid.tem" last no hash
#
# sert tempe hydro 1 9942 .05 grid 8575 6468 3606 776 304 169 103 66.2 44.1 31.3
#
# ism_grid.in
# class ism
# ======================================
```

this shows an S-curve calculation - make plot showing density as X-axis and gas pressure (nT) as y-axis

the gas is ionized by the galactic background. the density varies between 1e-3 and 100 cm-3. this is the full range found in the diffuse ism. The components that are produced are CNM - cold neutral medium, density ~ 40 cm-3 WNM - n ~ 0.5 cm-3, WIM - warm ionized medium, n ~ 0.25 cm-3 HIM - hot ionized medium, n ~ 1e-3 cm-3, calculation DOES NOT reproduce observed temperature of HIM - we get ~1e4K but observed is ~1e6 K. HIM is shock, not photo, ionized

---

`ism_hot_brems.in`

generate continuum due to hot ism in high Z,z starburst

```
title generate continuum due to hot ism in high Z,z starburst
set save prefix "ism_hot_brems"
#
# commands controlling continuum =========
# this sets up coronal equilibrium for temperature and continuum
# cloud is predominantly collisionally ionized
coronal equilibrium, t = 1.e6 K
#
# commands for density & abundances =========
# log of hydrogen density (cm-3), by default a constant density model
hden 1
# chemical composition for a well-evolved star cluster with high Z
# the starburst command generates scale factors that will be used to
# multiply the old solar composition, used in ver 84. this is maintain
# record of physical changes
abundances old solar 84
abundances starburst Z=10 Zsun
#
# commands controlling geometry =========
# the log of the total hydrogen column density, cm-2
stop column density 21
#
# other commands for details =========
# continuum is plotted in Hzay, we me must iterate to predict this
iterate
#
# commands controlling output =========
# normalize to O 7 Lya
normalize to "O 7" 21.6020
# this shortens the printout somewhat
print line faint 1
# output options
save performance ".per"
save continuum last ".con" no title, units keV
save sulphur ionization ".sul"
save overview last ".ovr"
save dr last ".dr"
#save species data sources ".dsource"
# this is only to document the problem described above
#
# ism_hot_brems.in
# class ism
```

```
# ======================================
#
```

This model generates a large column constant density cloud similar to the hot phase of the interstellar medium. The continuum is punched to generate one of the figures in Part 2 of Hazy.

There is a strange feature between 1.7e-3A and 2.2e-3A that is the N emission (head starting at 1.7e-3A with O absorption at 2.2e-3A. This model is strongly enriched in heavies so many metal edges, esp O, are optically thick.

>>TODO 1 the guess of the thickness of the first zone is badly too small, because this model is collisionally ionized, and it used Stromgren length - better to use collisional balance and dr - as result of this the model takes far too many zones

---

`ism_jura.in`

check rate H2 forms on grain surfaces

```
title check rate H2 forms on grain surfaces
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is hot star continuum
black 30000
intensity 1.90 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
cosmic rays, background
#
# commands for density & abundances =========
hden 0
grains ism, abundance log 0.16 no qheat
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
#
# commands controlling geometry =========
sphere
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
stop zone 1
#
# other commands for details =========
# set the gas temperature
constant temperature 100 K
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "c 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save overview "ism_jura.ovr"
save performance "ism_jura.per"
save hydrogen 21 cm last "ism_jura.21cm"
#
# ism_jura.in
# class limit
# ======================================
#
```

This model started out life as the Tielens & Hollenbach 1985 pdr. The density was set to unity and the incident radiation field adjusted so that the two default grains have temperatures near 100K. The model asserts that the H2 formation rate on grain surfaces is close to the # >>refer H2 grain physics Jura, M., 1975, ApJ, 197, 575 rate.

---

ism_opacity.in

generate standard ISM opacity curve

```
title generate standard ISM opacity curve
#
# commands controlling continuum =========
table agn
ionization parameter -3
#
# commands for density & abundances =========
grains no qheat
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "ism_opacity.ovr"
save performance "ism_opacity.per"
save total opacity last "ism_opacity.opc" units kev
#
# ism_opacity.in
# class limit
# ======================================
#
```

This example creates the file ism_opacity.opc which tabulates the total opacity of the gas as a function of energy. These plots are used in ISM studies to understand the transmission characteristics along a line of sight. The opacity depends on the dust to gas ratio, the gas phase abundances, and the level of ionization, all of which can be changed by altering parameters given above.

The model is of a 1 cm think parcel of gas which is optically thin in the Lyman continuum and Lyman lines. As a result the hydrogen emission line spectrum is close to case C. The model iterates so that the predicted ionization and emission know about this.

---

ism_set_cr_rate.in

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
cosmic ray rate -16
# this will be VERY faint black 50000
ionization parameter -25
black 50000
#
# commands for density & abundances =========
hden 5
element hydrogen ionization 1 0.00000001
#
```

```
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 1000 K
# turn off molecules to test only ions
# >>chng23 mar 04, add "heavy" option
no molecules heavy
# must turn off charge transfer and its heating, which would dominate,
# since we want to test cr heating and ionization
no charge transfer
no ctheat
# must turn of photoionization by recombining species,
# since we want to test cr heating and ionization
no photoionization
# any time photoionization is turned off, it is best to also
# turn off induced processes, which include pumping in the lyman lines
no induced processes
#
# commands controlling output =========
print ages
save overview "ism_set_cr_rate.ovr"
save performance "ism_set_cr_rate.per"
#
# ism_set_cr_rate.in
# class limit
# ======================================
#
```

This test conditions of cosmic ray ionization. Molecules and charge transfer are disabled so that analytical estimates can be made.

---

limit_casea_h_den13.in

case A

```
title case A
#
# Seaton, M.J, 1959 MN 119, 90,
# 4pi j(beta) 5.56E-26
# for this model total H-beta=4.745
# b(2)=3.73E-3 (3)=3.69E-2 (4)=0.091 (5)=0.145 (6)=0.193
# n.b. very different results if not l-mixed
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -2
#
# commands for density & abundances =========
init file="honly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature = 10000 K
iterate
#
# commands controlling output =========
# this should make the predicted totl Hbeta near unity for case a
normalize to "H 1" 4861.32A = 1.417
print populations h-like
```

```
print departure coefficients
save overview "limit_casea_h_den13.ovr"
save performance "limit_casea_h_den13.per"
#
# limit_casea_h_den13.in
# class limit
# ======================================
#
```

Case A is a mathematical fiction; when the Lyman lines are optically thin continuum pumping must be important if the gas is ionized. Fluorescence is turned off with the no induced processes command. The density is set to a very high value (1015 cm-3) so that the 2s-2p states are well l-mixed, in keeping with standard case A assumptions. As a result, collisional excitation would dominate the level populations, and hydrogen collisions must be turned off with the hydrogen collisions off command. The Ly* optical depth is set to a small value. The set dr command sets the zone thickness to 1 cm. The abundances are set to a very small value so that the electron density is equal to the hydrogen density.
Checks:
- Departure coefficients for H, He levels
- Neutral fractions
- H* emissivity

`limit_casea_h_den_temp.in`

Test model H in Case A limit

```
title Test model H in Case A limit
# grid over nebular range of density and temperature to check Case A H
#
# commands controlling continuum =========
# create H+
laser 2 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "honly.ini"
hden 2. vary
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no scattering escape
case A hummer no Pdest no photoionization
no induced processes
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 20
database H-like collapsed levels 30
save grid "limit_casea_h_den_temp.grd"
save overview "limit_casea_h_den_temp.ovr"
save performance "limit_casea_h_den_temp.per"
#
# fixit the wavelength range is adjusted to avoid the Lyman lines
# the Lyman a / 2 photon ratio is wrong at high Temperature -
# is there a temperature dependent branching ratio to n=2 out
# of the collapsed level?
#
# limit_casea_h_den_temp.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit. The grid is over both density and temperature.

---

limit_caseb_h_den10_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den10_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 10
set eden 10
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview ".ovr"
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den2_temp37.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
```

```
database h-like resolved levels 30
database h-like collapsed levels 70
database h-like keep fine structure
constant temper 3.7
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint -4
print line column
save overview "limit_caseb_h_den2_temp37.ovr"
save performance "limit_caseb_h_den2_temp37.per"
save diffuse continuum "limit_caseb_h_den2_temp37.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp37.con" last no title units microns
#
#
# limit_caseb_h_den2_temp37.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

`limit_caseb_h_den2_temp4.in`

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp4.ovr"
save performance "limit_caseb_h_den2_temp4.per"
save diffuse continuum "limit_caseb_h_den2_temp4.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp4.con" last no title units microns
#
#
```

```
# limit_caseb_h_den2_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_h_den2_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den2_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview ".ovr"
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den2_temp5.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
```

```
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temper 5
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp5.ovr"
save performance "limit_caseb_h_den2_temp5.per"
save diffuse continuum "limit_caseb_h_den2_temp5.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp5.con" last no title units microns
#
#
# limit_caseb_h_den2_temp5.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

`limit_caseb_h_den2_temp5_coronal.in`

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
coronal 5
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
# Hummer option not included here because the population of the excited states will be zero
case b no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp5_coronal.ovr"
save performance "limit_caseb_h_den2_temp5_coronal.per"
```

```
save diffuse continuum "limit_caseb_h_den2_temp5_coronal.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp5_coronal.con" last no title units microns
```

---

limit_caseb_h_den4_temp4.in

```
set save prefix "limit_caseb_h_den4_temp4"
#
# Gary tripped over a bug when this command is issued before
# the 'init "honly.ini"' below.
# Keep this command up here to always exercise the fix.
#
save species bands ".band" "FeII_bands.ini" "Fe+"
constant temperature 1e4
hden 4
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den4_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 10000 linear
set eden 4
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview ".ovr"
```

```
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den4_temp4_Fuji.in

```
set save prefix "limit_caseb_h_den4_temp4_Fuji"
constant temperature 1e4
hden 4
database collisions h-like hydrogen Fujimoto
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp4_VR62.in

```
set save prefix "limit_caseb_h_den4_temp4_VR62"
constant temperature 1e4
hden 4
database collisions h-like hydrogen van regemorter
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp4_VS80.in

```
set save prefix "limit_caseb_h_den4_temp4_VS80"
constant temperature 1e4
hden 4
database collisions h-like hydrogen vriens
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
```

```
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_hs87.in

"Case B from Hummer and Storey"

```
title "Case B from Hummer and Storey"
init "honly.ini"
laser 1.1
ionization parameter -1
constant temperature 4
case b hummer no photoionization no pdest
database h-like element hydrogen levels resolved 40
database h-like element hydrogen collapsed levels 70
no induced processes
no level2
no scattering escape
set dr -20
hden 4
stop zone 1
iterate
print populations h-like
print departure h-like
save overview "limit_caseb_h_hs87.ovr"
save performance "limit_caseb_h_hs87.per"
#
#
# limit_caseb_h_hs87.in
# class limit
```

---

limit_caseb_h_lot.in

log density case B, T=500 log n=2

```
title log density case B, T=500 log n=2
#
# commands controlling continuum =========
black body, T = 2.e5 K
ionization parameter -1
#
# commands for density & abundances =========
hden = 2
init file="honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature = 500
# want H and he fully stripped so we can check H He spectra
case b hummer no photoionization no pdest
no induced processes (OK)
iterate
#
# commands controlling output =========
#
```

```
# does not agree with Hummer & Storey, as explained by Ferguson & Ferland
# until 03 jun 02, used small atom, which had smaller differences
# turn on large atom to get best answer
database h-like levels resolved 20
#
save overview "limit_caseb_h_lot.ovr"
save performance "limit_caseb_h_lot.per"
save results "limit_caseb_h_lot.rlt" last
#
```

limit_caseb_h_lot.in # class limit # ===

This tests the ionization and emission line spectrum for H case B at a low density and temperature.

`limit_caseb_h_n8.in`

h_caseb_n8 high density case B

```
title h_caseb_n8 high density case B
#
# commands controlling continuum =========
black body, T = 2.e5 K
ionization parameter -1
#
# commands for density & abundances =========
hden = 8
init file="honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
# this will not affect the main model, but will test CR heating rate
cosmic ray background
case b hummer no photoionization no Pdest
no scattering escape
no induced processes (OK)
constant temperature = 20000
iterate
database h-like resolve levels 20
#
# commands controlling output =========
save overview "limit_caseb_h_n8.ovr"
save performance "limit_caseb_h_n8.per"
save results "limit_caseb_h_n8.rlt"
save ionizing continuum "limit_caseb_h_n8.cion"
#
#
# limit_caseb_h_n8.in
# class limit
# =======================================
#
```

This test case compares the predictions of the multi-level hydrogen atom with the Storey and Hummer (1995) results. The set dr command sets the zone thickness to 1 cm. The case b command sets Lyman line optical depths to very large values. Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities

high density causes disagreemeent with HS - collisions

---

limit_caseb_he2_den8.in

limit_caseb_he2_den8 He II case B

```
title limit_caseb_he2_den8 He II case B
#
# commands controlling continuum =========
table agn
ionization parameter 0
#
# commands for density & abundances =========
hden = 8
element helium abundance 1
init file="ism.ini"
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
database h-like element helium levels resolved 30
case b hummer no photoionization no Pdest
no induced processes (OK)
constant temperature = 5e4 K
#
# commands controlling output =========
save overview "limit_caseb_he2_den8.ovr"
save performance "limit_caseb_he2_den8.per"
save results "limit_caseb_he2_den8.rlt"
#
#
# limit_caseb_he2_den8.in
# class limit
# ======================================
#
```

This test case compares the predictions of the multi-level hydrogen atom with the Storey and Hummer (1995) results. The set dr command sets the zone thickness to 1 cm. The case b command sets Lyman line optical depths to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities

---

limit_caseb_he_den.in

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
laser 5 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
```

```
# other commands for details =========
normalize to "He 2" 4685.68A
case b hummer no Pdest no photoionization
no scattering escape
# prevent H I excited levels from being predicted
database H-like element hydrogen resolved levels 3
constant temperature 4.
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 15
save grid "limit_caseb_he_den.grd"
save overview "limit_caseb_he_den.ovr"
save performance "limit_caseb_he_den.per"
#
#
# limit_caseb_he_den.in
# class limit
# ======================================
#
```

this tests the predicted He II spectra in the Case B limit.

this effectively turns off hydrogen to avoid the problem with every other heII line lying beneath an HI line. this is done by reducing the number of levels for H I.

this asserts the values are within 9% for the standard T = 1e4K and a range of densities. Actually they are all nearly within a few percent except at the lowest temperature of 5000K.

`limit_caseb_he_den2_temp4.in`

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 90 linear
set eden 2
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -2.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database he-like gbar vriens
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den2_temp4.fit"
save overview "limit_caseb_he_den2_temp4.ovr"
```

```
save performance "limit_caseb_he_den2_temp4.per"
save diffuse continuum "limit_caseb_he_den2_temp4.dif" last no title units microns
save continuum "limit_caseb_he_den2_temp4.con" last no title units microns
save line list ratio column "limit_caseb_he_den2_temp4.rat" "linelist_he1.dat" last no hash
#
save line populations "limit_caseb_he_den2_temp4.lpop" "linelist_he1.dat" last no hash
# default row option: ratio
save line populations "limit_caseb_he_den2_temp4.row.lpop" "linelist_he1.dat" row last no hash
save line populations "limit_caseb_he_den2_temp4.row_lower.lpop" "linelist_he1.dat" row lower last no
hash
save line populations "limit_caseb_he_den2_temp4.row_upper.lpop" "linelist_he1.dat" row upper last no
hash
save line populations "limit_caseb_he_den2_temp4.row_ratio.lpop" "linelist_he1.dat" row ratio last no
hash
save line populations "limit_caseb_he_den2_temp4.row_tspin.lpop" "linelist_he1.dat" row tspin last no
hash
#
#
# limit_caseb_he_den2_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

`limit_caseb_he_den4_temp4.in`

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database he-like gbar vriens
constant temper 4
case b hummer no photoionization no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den4_temp4.fit"
save overview "limit_caseb_he_den4_temp4.ovr"
save performance "limit_caseb_he_den4_temp4.per"
save diffuse continuum "limit_caseb_he_den4_temp4.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4.con" last no title units microns
```

```
save line list ratio column "limit_caseb_he_den4_temp4.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4_Fuji.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium Fujimoto
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
save overview "limit_caseb_he_den4_temp4_Fuji.ovr"
save performance "limit_caseb_he_den4_temp4_Fuji.per"
save diffuse continuum "limit_caseb_he_den4_temp4_Fuji.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4_Fuji.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_Fuji.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4_VR62.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium van regemorter
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
save overview "limit_caseb_he_den4_temp4_VR62.ovr"
save performance "limit_caseb_he_den4_temp4_VR62.per"
save diffuse continuum "limit_caseb_he_den4_temp4_VR62.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4_VR62.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_VR62.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

`limit_caseb_he_den4_temp4_VS80.in`

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
```

```
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium Vriens
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den4_temp4.fit"
save overview "limit_caseb_he_den4_temp4_VS80.ovr"
save performance "limit_caseb_he_den4_temp4_VS80.per"
save diffuse continuum "limit_caseb_he_den4_temp4_VS80.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4_VS80.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_VS80.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

`limit_caseb_he_den_temp.in`

Test model He atoms in Case B limit

```
title Test model He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
laser 5 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 6 2 -2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
normalize to "He 2" 4685.68A
case b hummer no Pdest no photoionization
no scattering escape
# prevent H I excited levels from being predicted
database H-like element hydrogen resolved levels 3
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 20
```

```
save grid "limit_caseb_he_den_temp.grd"
save overview "limit_caseb_he_den_temp.ovr"
save performance "limit_caseb_he_den_temp.per"
#
#
# limit_caseb_he_den_temp.in
# class limit
# ======================================
#
```

this tests the predicted He II spectra in the Case B limit.

this effectively turns off hydrogen to avoid the problem with every other heII line lying beneath an HI line. this is done by reducing the number of levels for H I.

this asserts the values are within 15% for a range of density and temperature. Actually they are all nearly within a few percent except at the lowest temperature. The error greater than 10% occurs at the lowest temperature of 5000K.

`limit_caseb_hhe_den.in`

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
# create H+ and He+
laser 2.0 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
print line precision 5
database he-like element helium resolved levels 10
no scattering escape
case b hummer no Pdest no photoionization
constant temperature 4.
#
# commands controlling output =========
database H-like print levels
save grid "limit_caseb_hhe_den.grd"
save overview "limit_caseb_hhe_den.ovr"
save performance "limit_caseb_hhe_den.per"
#
# Case B helium doesn't work well with Hummer option
#
# limit_caseb_hhe_den.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit.

the grid is over density at the standard temperature of 1e4 K.

---

limit_caseb_hhe_den_temp.in

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
# create H+ and He+
laser 2 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 2 6 2 ncpus 4
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
print line precision 5
database he-like element helium resolved levels 10
database h-like element hydrogen resolved levels 15
no scattering escape
case b hummer no Pdest no photoionization
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
save grid "limit_caseb_hhe_den_temp.grd"
save overview "limit_caseb_hhe_den_temp.ovr"
save performance "limit_caseb_hhe_den_temp.per"
#
# Case B helium doesn't work well with Hummer option
#
# limit_caseb_hhe_den_temp.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit. The grid is over both density and temperature.

---

limit_casec_h_den2.in

H only optically thin in Lyman continuum

```
title H only optically thin in Lyman continuum
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands controlling geometry =========
stop thickness 16
#
# commands for density & abundances =========
hden 2
init file "honly.ini"
#
# other commands for details =========
iterate
```

```
constant temper 10000
no level2
#
# commands controlling output =========
print line inward
save performance "limit_casec_h_den2.per"
save overview "limit_casec_h_den2.ovr" last
save fine optical depths last "limit_casec_h_den2.fin" range 0.9 1.02 every 1
save optical depths last "limit_casec_h_den2.opt"
save continuum "limit_casec_h_den2.con" last units microns
save dr "limit_casec_h_den2.dr" last
#
# limit_casec_h_den2.in
# class limit
# ======================================
#
```

This is a pure hydrogen cloud that is optically thin in the Lyman continuum. The asserts check the emission in several H I lines and continua. This should be close to what really happens in a low column density cloud exposed to a continuum source that does not have strong Lyman lines. (The continuum source used is a pure blackbody, and so has no lines). So this is an example of "Case C" emission >>refer H case C Ferland, G.J. 1999, PASP, 111, 1524

`limit_casec_h_den5.in`

case C

```
title case C
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -2
#
# commands for density & abundances =========
hden = 5
init file="hheonly.ini"
#
# commands controlling geometry =========
set dr -10
stop zone 1
#
# other commands for details =========
iterate
stop lyman optical depth -6
constant temperature = 10000 K
#
# commands controlling output =========
print h-like populations element hydrogen
print line pump
print departure coefficients element hydrogen
save overview "limit_casec_h_den5.ovr"
save performance "limit_casec_h_den5.per"
#
# limit_casec_h_den5.in
# class limit
# ======================================
#
```

This is Case C, what really happens when optically thin gas is irradiated by a continuum with Lyman line continuum fluorescence allowed.
Checks:
- Departure coefficients for H, He levels
- Neutral fractions
- H* emissivity Case C is described in

>>refer H case C Ferland, G.J. 1999, PASP, 111, 1524

---

limit_compton_hi_t.in

test high-T Compton energy exchange

```
title test high-T Compton energy exchange
#
# commands controlling continuum =========
# as hot as STE bb can be on IEEE 32-bit cpu
# equilibrium temperature should also be 2.51e7
# since gas radiated by true blackbody will equilibriate
# at its temperature
blackbody 7.4 STE
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database h-like element oxygen resolved levels 5
database h-like element oxygen collapsed levels 30
set temperature convergence 0.0001
iterate
print h-like departure element oxygen
#
# commands controlling output =========
save overview "limit_compton_hi_t.ovr"
save performance "limit_compton_hi_t.per"
#
# limit_compton_hi_t.in
# class limit
# ======================================
#
```

This is the highest Compton temperature that can be computed in LTE on an IEEE 32-bit processor. This tests the code in the high-temperature Compton limit. Temperatures as high as 10^10 K can be computed successfully on CPUs with longer word lengths, such as a Cray or the new 64 bit processors.

Checks:
- The equilibrium temperature should be exactly 107.4 K (2.51239107 K).

---

limit_compton_lo_t.in

test low-T Compton energy exchange

```
title test low-T Compton energy exchange
#
# commands controlling continuum =========
black linear 3 lte
brems 5
ionizat -5
#
# commands for density & abundances =========
hden -10
init file "hheonly.ini"
eden -3
```

```
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
set temperature convergence 0.0001
iterate 3
#
# commands controlling output =========
save overview "limit_compton_lo_t.ovr"
save performance "limit_compton_lo_t.per"
#
# limit_compton_lo_t.in
# class limit
# ======================================
#
```

This tests the code in the low temperature Compton limit. The gas is illuminated by a 3 K blackbody in thermodynamic equilibrium. The equilibrium temperature should be exactly 3 K. It is necessary to add an extra component of free electrons to test the code in this limit with the eden command. If eden is pushed up too high, ee brems cooling will be artificially boosted compared to other cooling terms and start cooling the gas below 3 K. This is why eden was set to 1e-3 cm^-3 on 20141105.

`limit_compton_mid_t.in`

mid-T Compton energy exchange

```
title mid-T Compton energy exchange
# test of thermal equil in limit_compton_mid_t limit; temp should EXACTLY equal 2E5K
# check continuum partition;
# energy range, photon densities, luminosities, follow
# 0.25-1. Q=26.6470 L=15.8190 c 1-1.807 Q=26.8867 L=16.3766
# 1.807-4 Q=27.3042 L=17.0948 c 4-20 Q=27.2041 L=17.3179
# 20 -- Q=22.9038 L=22.9038 c total lumin 17.5597
# nufnu(912A) = 1.8029E+16
#
# commands controlling continuum =========
black body t = 2.e5 K lte
#
# commands for density & abundances =========
hden = 6
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
stop lyman continuum optical depth = -6
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
print line faint .1
print departure coef element hydrogen
save overview "limit_compton_mid_t.ovr"
save performance "limit_compton_mid_t.per"
#
# limit_compton_mid_t.in
# class limit
# ======================================
#
```

This tests the behavior of the code in the Compton limit. The incident continuum is a blackbody in strict thermodynamic equilibrium. Strict thermodynamic equilibrium is expected for all constituents of the gas. The input stream also lists the

expected photon fluxes for the incident continuum; this tests the normalization of the continuum, and its distribution. Grains are included to confirm their behavior in the LTE limit. The set dr command sets the zone thickness to 1 cm.

Checks:
- Luminosity, photon flux, over various energy intervals, 4*J at 912143.
- Electron temperature exactly 2*105 K.
- Grain temperature forced to 2*105 K by radiative processes.

`limit_conserve.in`

test that energy is limit_conserved

```
title test that energy is limit_conserved
#
# commands controlling continuum =========
# primary continuum is a hot blackbody
black body, temp=5.5
intensity total -4
# add cosmic background
background
#
# commands controlling geometry =========
# don't stop the calculation until all energy used up
# in order to check energy conservation
stop temperature 3 linear
# cloud will go very deep with temperature near 3K without this
stop thickness 18.1
#
# commands for density & abundances =========
metals -0.5
hden 1.0
constant pressure
#
# other commands for details =========
iterate
# want a clean calculation
failures 3
# this allows for more molecular gas beyond what we model
double optical depths
#
# commands controlling output =========
save performance "limit_conserve.per"
save pressure "limit_conserve.pre"
save pressure history "limit_conserve.his"
save cooling "limit_conserve.col"
save heating "limit_conserve.het"
save dr "limit_conserve.dr"
save overview "limit_conserve.ovr1"
save overview last "limit_conserve.ovr"
save results "limit_conserve.rlt"
save element carbon "limit_conserve.car"
save element neon "limit_conserve.ne"
save element magnesium "limit_conserve.mag"
save element silicon "limit_conserve.sil"
#
# limit_conserve.in
# class hii pdr
# ======================================
```

This checks that energy is limit_conserved. The code always checks that it did not radiate more energy than was absorbed. This calculation extends well past the photo-dissociation zone into fully molecular gas, so that all of the incident radiation is absorbed. Grains, CMB, & CRs are not present so that only the incident radiation field powers the gas.

Small changes can affect this model to surprising extents because of the presence of a major thermal front at the H0 - H+ transition region.

---

limit_eden.in

Martin Gaskell's funny model

```
title Martin Gaskell's funny model
# used to test that electron density convergence is ok
# hydrogen line spectrum strongly pumped by continuum
# all elements > H have HIGH abundances
# ionization of elements Fe, Mg, Si strongly affected
# by charge transfer
#
# commands controlling continuum =========
black 4000
lumin 27.2
#
# commands for density & abundances =========
hden 5.138
abundances all 1000
#
# commands controlling geometry =========
radius 15
stop zone 1
set dr 0
#
# other commands for details =========
constant temper 5500
#
# commands controlling output =========
print line faint -3
save overview "limit_eden.ovr"
save performance "limit_eden.per"
#
# limit_eden.in
# class limit
# ======================================
#
```

This is mainly a test of the ability of the code to converge a model with a very strange electron density. The electrons are mainly contributed by heavy elements, and the gas is only slightly ionized.

Ionization of elements Fe, Mg, Si strongly affected by charge transfer with other heavy elements.

Checks:
- Electron density is correct.
- Hydrogen line spectrum strongly pumped by continuum.

---

limit_h_induc.in

constant temper black body limit from Ferland and Rees 1988

```
title constant temper black body limit from Ferland and Rees 1988
# tests whether departure coef are forced to unity by induced processes
#
# commands controlling continuum =========
black body, t = 50000 lte
#
```

```
# commands for density & abundances =========
hden 10
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman continuum optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
constant temper 50000
#
# commands controlling output =========
print populations h-like element hydrogen
print heating
print departure coef element hydrogen
print line faint -1
save overview "limit_h_induc.ovr"
save performance "limit_h_induc.per"
#
# limit_h_induc.in
# class limit
# ======================================
#
```

This example tests whether induced processes force level populations of hydrogen to LTE when they are irradiated by a blackbody in strict thermodynamic equilibrium. The density is low enough value for radiation to dominate the rate equations coupling levels with each other and the continuum. The expectation is for all departure coefficients to equal unity.

Checks:
- Departure coefficients exactly unity.
- Grain temperatures are exactly 5*104 K.

`limit_hi_ion.in`

very high ionization parameter limit

```
title very high ionization parameter limit
# commands controlling continuum =========
table agn
ionization parameter 15
# commands controlling geometry =========
hden 0
stop zone 1
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "limit_hi_ion.ovr"
save performance "limit_hi_ion.per"
save heating "limit_hi_ion.het"
save cooling "limit_hi_ion.col"
#
#
# func_hi_ion.in
# class function
# ======================================
#
```

This tests a limit of very high ionization

---

limit_laser_1.in

test of H ionization in optically thin limit

```
title test of H ionization in optically thin limit
#
# commands controlling continuum =========
laser 1.5 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
init file="hheonly.ini"
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature = 4
iterate to convergence
#
# commands controlling output =========
save overview "limit_laser_1.ovr"
save performance "limit_laser_1.per"
save convergence reason "limit_laser_1.cvr"
#
# limit_laser_1.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen photoionization equilibrium. The continuum is a laser peaked at 1.5 Ryd, where the hydrogen photoionization cross section is 2.09*10-18 cm-2.

Checks:
- The hydrogen neutral fraction is nearly 2.00*10-4 (not exact since laser has finite width).
- Hb emissivity close to high density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.

H cross section is 2.09E-18 cm^2, rec coef is 4.18E-14 answer is neutral fraction 2.00E-4 also checks that only 3 iterations needed

---

limit_laser_2.in

test of H and HeI ionization in optically thin limit

```
title test of H and HeI ionization in optically thin limit
#
# commands controlling continuum =========
laser 2.0 Ryd
intensity -0.3604
#
# commands for density & abundances =========
hden 1
init file="hheonly.ini"
abundances all -10
#
# commands controlling geometry =========
stop zone 1
```

```
set dr 0
#
# other commands for details =========
constant temperature = 4
iterate to convergence
#
# commands controlling output =========
save overview "limit_laser_2.ovr"
save performance "limit_laser_2.per"
#
# limit_laser_2.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen and helium photoionization equilibrium. The continuum is a laser peaked at 2.0 Ryd, and so can only ionize hydrogen and atomic helium.

Checks:
- The hydrogen neutral fraction is nearly Ho/H+=4.51*10-4 (not exact since laser has finite width).
- Hb emissivity close to high density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.
- Helium ionization should be Heo/He+ = 6.61*10-4.

H cross section is 0.927E-18 cm^2, rec coef is 4.18E-13 answer is Ho/H+ = 4.51e-4 HeI cross section is 6.54E-18 cm^2, rec coef is 4.32E-13 answer is Heo/He+ = 6.61e-5

`limit_laser_200.in`

ionization in Auger-dominated limit

```
title ionization in Auger-dominated limit
#
# commands controlling continuum =========
laser 200 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 5
#
# commands controlling output =========
save overview "limit_laser_200.ovr"
save performance "limit_laser_200.per"
#
# limit_laser_200.in
# class limit
# ======================================
#
```

This checks the calculation of ionization equilibrium. The continuum is a laser peaked at 200 Ryd. It asserts ionization of C, O, and Fe. their ionization is dominated by the Auger effect.

Checks: Auger OK

limit_laser_200_low.in

test ionization in Auger-dominated limit

```
title test ionization in Auger-dominated limit
#
# commands controlling continuum =========
laser 200 Ryd
phi(h) 5
#
# commands for density & abundances =========
hden 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 4
#
# commands controlling output =========
save overview "limit_laser_200_low.ovr"
save performance "limit_laser_200_low.per"
#
#
#
#
#
# limit_laser_200_low.in
# class limit
# ========================================
#
```

This checks the calculation of ionization equilibrium. The continuum is a laser peaked at 200 Ryd. It asserts ionization of C, O, and Fe. their ionization is dominated by the Auger effect.

Checks: Auger OK

---

limit_laser_3.in

test H and He ionization in optically thin limit

```
title test H and He ionization in optically thin limit
#
# commands controlling continuum =========
laser 4.3 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
abundances all -10
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 4
```

```
#
# commands controlling output =========
save overview "limit_laser_3.ovr"
save performance "limit_laser_3.per"
#
# limit_laser_3.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen and helium photoionization equilibrium. The continuum is a laser peaked at 4.3 Ryd, where it can fully ionize both hydrogen and helium.

Checks:
- The hydrogen neutral fraction is nearly 4.18*10-4 (not exact since laser has finite width).
- Helium ion: The ratio He+/He++ should be 1.69*10-3 and the ratio Heo/He+ should be 2.86*10-4.
- Hb emissivity should be close to high-density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.

H cross section is 1.0E-18 cm^2, rec coef is 4.18E-13 answer is n(Ho)/n(H+)=4.18e-3 HeI cross section is 1.51E-18 cm^2, rec coef is 4.32e-13 answer is n(Heo)/n(He+)=2.86e-4, so Heo/He = 4.83e-7 HeII cross section is 1.30E-18 cm^2, rec coef is 2.20e-12 answer is n(He+)/n(He2+)=1.69e-3

`limit_lowd0.in`

test low density limit

```
title test low density limit
# this and limit_lowdm6 should get same results
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 0
abundances old solar 84
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "H 1" 4861.32A 0.86
print line sort wavelength range 100 1m
save overview "limit_lowd0.ovr"
save performance "limit_lowd0.per"
save cooling last "limit_lowd0.col"
save continuum last "limit_lowd0.con"
#
# all asserts for both sims are in this file
init file="lowd.dat"
#
# limit_lowd0.in
# class limit
# ======================================
#
```

this test case is paired with lowdm6.in both tests read in the same set of asserts, those contained in the file lowd.dat, and they should get exactly the same answer

this is also the test of the print lines intensity command

`limit_lowden.in`

test optically thin model that extends to very low densities

```
title test optically thin model that extends to very low densities
#
# commands controlling continuum =========
table agn
ionization parameter 0
#
# commands for density & abundances =========
hden -2 to the -2 power
init file="ism.ini"
#
# commands controlling geometry =========
sphere
# this will take density down to 1e-8, below stated limit
radius 10 13
#
# other commands for details =========
#
# commands controlling output =========
save performance "limit_lowden.per"
save overview "limit_lowden.ovr" last
#
# limit_lowden.in
# class limit
# ======================================
#
```

This model is optically thin, with density falling off as inverse square law, so ionization and temperature should be nearly constant. if outer radius increased by 2 dex problem with level3 will appear, several li seq lines (OVI, NeVIII) will fluctuate when density about 1e-9

We do not assert H lines since the cloud is optically thin and takes at least three iterations to converge optical depth scale, That is not the purpose of this sim

---

`limit_lowdm6.in`

test low density limit

```
title test low density limit
# this and limit_lowd0 should get same results
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden -6
abundances old solar 84
#
# commands controlling geometry =========
stop zone 1
set dr 0
```

```
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "H 1" 4861.32A 0.86
print line sort wavelength range 100 1m
save overview "limit_lowdm6.ovr"
save performance "limit_lowdm6.per"
save cooling last "limit_lowdm6.col"
save continuum last "limit_lowdm6.con"
#
# all asserts are in this file
init file="lowd.dat"
#
# limit_lowdm6.in
# class limit
# ======================================
#
```

this test case is paired with lowd0.in both tests read in the same set of asserts, those contained in the file lowd.dat, and they should get exactly the same answer

this also tests the print line sort range command

`limit_lowion.in`

test conditions of very low ionization matrix solver

```
title test conditions of very low ionization matrix solver
#
# commands controlling continuum =========
blackbody 50000
ionization parameter -30
#
# commands for density & abundances =========
hden 2
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
constant temperature 100
#
# commands controlling output =========
save overview "limit_lowion.ovr"
save performance "limit_lowion.per"
#
# limit_lowion.in
# class limit
# ======================================
#
```

This model test very low ionization solution of hydrogen and helium.

`limit_lte_h_t50_cion.in`

collisionally ionized H in LTE limit

```
title collisionally ionized H in LTE limit
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -8
#
# commands for density & abundances =========
hden = 20
set eden 20
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
constant temperature = 50000 K
# want pure collisional model
no induced processes (OK)
database h-like collisional excitation off
database h-like collisions l-mixing off
database he-like collisional excitation off
database he-like collisions l-mixing off
database he-like collapsed levels 20
iterate
#
# commands controlling output =========
print h-like departure coefficients hydrogen
print he-like departure coefficients helium
print populations h-like hydrogen
save overview "limit_lte_h_t50_cion.ovr"
save performance "limit_lte_h_t50_cion.per"
#
# limit_lte_h_t50_cion.in
# class limit
# ========================================
#
```

This is the limiting case pure hydrogen collisional ionization, There are no excitation or l-mixing collisions, so this tests whether collisional ionization - three body recombination works in detailed balance.

`limit_lte_h_t50_coll.in`

collisionally excited H in LTE limit

```
title collisionally excited H in LTE limit
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -8
#
# commands for density & abundances =========
hden = 20
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
stop zone 1
set dr 0
set eden 20
#
# other commands for details =========
no induced processes (OK)
```

```
database h-like collisions l-mixing off
database he-like collapsed levels 20
database he-like collisions l-mixing off
constant temperature = 50000 K
iterate
#
# commands controlling output =========
print h-like departure coefficients hydrogen
print h-like populations hydrogen
print he-like departure coefficients helium
save overview "limit_lte_h_t50_coll.ovr"
save performance "limit_lte_h_t50_coll.per"
#
# limit_lte_h_t50_coll.in
# class limit
# ======================================
#
```

This checks that the model H atom goes to LTE at high densities.

chng 06 aug 24, had not included collisional ionization, and so he-like departure coefficients were very large, around 202. comments said there were problems. turned on collisional ionization, no problems noted

chng 06 jul 22 with RP changes in high-n n-changing collisions the rates are now much smaller - needed to change density to be far higher and several quantities changed. at lower density (1e18 cm-3) the populations are very unphysical and runaway maser now occurs. this is only a homework problem and intended to only test n-changing collisions. with higher density this test is done.

`limit_lte_he1_coll.in`

He atom at high densities

```
title He atom at high densities
#
# commands controlling continuum =========
laser 2
ionization -3
#
# commands for density & abundances =========
hden 18
set eden 18
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -10
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 20000 K
iterate
#
# commands controlling output =========
print he-like departure helium
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_coll.ovr"
save performance "limit_lte_he1_coll.per"
#
# limit_lte_he1_coll.in
# class limit
```

```
# ======================================
#
```

test whether he-like ion populations go to lte in high density limit. The level populations should be in LTE, and the departure coefficients should be unity.

---

limit_lte_he1_nomole_iso_force.in

He atom in LTE at high densities, with no molecules, iso forced to LTE

```
title He atom in LTE at high densities, with no molecules, iso forced to LTE
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
# atom he-like levels 7
# atom he-like collapsed levels 30
no molecules
database h-like levels LTE
database he-like levels LTE
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_iso_force.ovr"
save performance "limit_lte_he1_nomole_iso_force.per"
save heating "limit_lte_he1_nomole_iso_force.het"
save cooling "limit_lte_he1_nomole_iso_force.col"
save dr "limit_lte_he1_nomole_iso_force.dr"
#
# limit_lte_he1_nomole_iso_force.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

---

limit_lte_he1_nomole_ste.in

He atom in LTE at high densities, with no molecules

```
title He atom in LTE at high densities, with no molecules
#
# commands controlling continuum =========
```

```
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 7
database he-like collapsed levels 30
no molecules
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_ste.ovr"
save performance "limit_lte_he1_nomole_ste.per"
save heating "limit_lte_he1_nomole_ste.het"
save cooling "limit_lte_he1_nomole_ste.col"
save dr "limit_lte_he1_nomole_ste.dr"
save species departure "limit_lte_he1_nomole_ste.dep" last all
#
# limit_lte_he1_nomole_ste.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

`limit_lte_he1_nomole_ste_nocoll.in`

He atom in LTE at high densities, with no molecules and no collapsed levels

```
title He atom in LTE at high densities, with no molecules and no collapsed levels
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
```

```
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_ste_nocoll.ovr"
save performance "limit_lte_he1_nomole_ste_nocoll.per"
save heating "limit_lte_he1_nomole_ste_nocoll.het"
save cooling "limit_lte_he1_nomole_ste_nocoll.col"
save dr "limit_lte_he1_nomole_ste_nocoll.dr"
#
# limit_lte_he1_nomole_ste_nocoll.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

Level collapse options have been switched off in this, compared to limit_lte_he1_nomole_ste, so effect of including the collapsed levels on LTE can be verified.

`limit_lte_he1_nomole_ste_nocoll2.in`

He atom in LTE for a large range of Te and density, with no molecules and no collapsed levels and no collisions

```
title He atom in LTE for a large range of Te and density, with no molecules and no collapsed levels
and no collisions
#
# commands controlling continuum =========
blackbody 4.3 STE vary
grid 3.7 to 6.5 step 0.1 sequential
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18 vary
grid 4 to 18 2.0
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
database h-like collisions off
database he-like collisions off
set dr -10
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
normalize to "Inci" 4860
print line faint -2
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save grid "limit_lte_he1_nomole_ste_nocoll2.grd"
save overview "limit_lte_he1_nomole_ste_nocoll2.ovr"
save performance "limit_lte_he1_nomole_ste_nocoll2.per"
save heating "limit_lte_he1_nomole_ste_nocoll2.het"
save cooling "limit_lte_he1_nomole_ste_nocoll2.col"
```

```
save dr "limit_lte_he1_nomole_ste_nocoll2.dr"
#
# >>chng 14 dec 14, Badnell S DR, increase error
# limit_lte_he1_nomole_ste_nocoll2.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in a range of conditions. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

These are STE calculations with no collapsed levels, no collisions, and no molecules, so these models should stringently test the thermodynamic equilibrium limit of radiative coupling terms.

---

limit_lte_he1_ste.in

He atom in LTE at high densities

```
title He atom in LTE at high densities
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 18
# a high he abundance so that it dominates
element helium abundance 1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 7
database he-like collapsed levels 30
# atom h2 matrix all
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_ste.ovr"
save performance "limit_lte_he1_ste.per"
save heating "limit_lte_he1_ste.het"
save cooling "limit_lte_he1_ste.col"
save dr "limit_lte_he1_ste.dr"
save species departure "limit_lte_he1_ste.dep" last all
save dominant rates "limit_lte_he1_ste.h2" "H2"
#
# limit_lte_he1_ste.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

---

limit_lte_hhe_coll_t50.in

H, He in LTE at high densities

```
title H, He in LTE at high densities
# test from Ferland and Rees 88, collisions drive H to LTE
# collisions should drive all departure coef to unity
#
# commands controlling continuum =========
black body t = 50000
ionization parameter -5
#
# commands for density & abundances =========
hden = 19
init file="hheonly.ini"
set eden 20
#
# commands controlling geometry =========
set dr -10
stop zone 1
stop lyman optical depth -6
#
# other commands for details =========
constant temperature = 50000
iterate
#
# commands controlling output =========
print departure coefficients h-like hydrogen
print populations h-like hydrogen
print departure coefficients h-like helium
print populations h-like helium
print departure coefficients he-like helium
print populations he-like
save overview "limit_lte_hhe_coll_t50.ovr"
save performance "limit_lte_hhe_coll_t50.per"
save dr "limit_lte_hhe_coll_t50.dr" last
#
# limit_lte_hhe_coll_t50.in
# class limit
# ======================================
#
```

This model is a test of the behavior of hydrogen and helium in the high density, collision dominated, limit. The temperature is preset, the hydrogen density is set to a very high value, and the ionization parameter is very low. The resulting model is collision dominated, so this case checks that the collision physics occurs in detailed balance. The predicted departure coefficients should all equal unity. The set dr command sets the zone thickness to 1 cm.

Checks:
- Hydrogen departure coefficients exactly unity.
- Helium departure coefficients near unity. (Density not high enough to bring helium departure coefficients exactly to unity.)
- H-, H2, H2+ H3+, and HeH+ departure coefficients exactly unity. `

`limit_lte_hhe_induc.in`

radiation dominated H, He gas goes to STE

```
title radiation dominated H, He gas goes to STE
#
# commands controlling continuum =========
black body, t = 50000 STE
#
```

```
# commands for density & abundances =========
hden 4
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman continuum optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
set temperature convergence 0.002
#
# commands controlling output =========
print populations h-like hydrogen
print heating
print departure coef element hydrogen
print line faint -1
save overview "limit_lte_hhe_induc.ovr"
save performance "limit_lte_hhe_induc.per"
#
# limit_lte_hhe_induc.in
# class limit
# ========================================
#
```

This is a H, He-only gas that is optically thin in the Lyman continuum. It is irradiated by a blackbody in strict thermodynamic equilibrium. The tests confirm that the gas temperature equilibriates close to the black body temperature.

`limit_lte_hhe_ste.in`

H, He in STE

```
title H, He in STE
# from Ferland and Rees 1988
# this tests whether thermal processes go to STE
#
# commands controlling continuum =========
black body, t = 50000 STE
#
# commands for density & abundances =========
hden 10
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
print heating
print populations h-like hydrogen
print departure coef h-like hydrogen
print departure coef he-like helium
save overview "limit_ste_hhe_ste.ovr"
save performance "limit_ste_hhe_ste.per"
#
# limit_ste_hhe_ste.in
# class limit
# ========================================
#
```

This is the ultimate test of the behavior of the code in the strict thermodynamic equilibrium limit. The temperature is not held constant, so the resulting equilibrium temperature determines whether cooling processes are treated properly in the detailed balance limit. The equilibrium temperature should be exactly 5*104 K, and all departure coefficients should equal unity. A small amount of grains are included to check that the grain thermal balance is handled properly in this limit.

Checks:
- Electron temperature exactly 5*104 K.
- Departure coefficients unity.

---

limit_lte_hminus.in

H- goes to LTE

```
title H- goes to LTE
#
# commands controlling continuum =========
# this is a second way to get STE and tests the energy density option
blackbody 5000 energy density 5000K
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
constant temperature 5000
#
# commands controlling output =========
print populations h-like hydrogen
save overview "limit_lte_hminus.ovr"
save performance "limit_lte_hminus.per"
print departure coef element hydrogen
#
# limit_lte_hminus.in
#
# class limit
# ========================================
#
```

This checks that the negative hydrogen ion goes to thermodynamic equilibrium when irradiated by a blackbody in thermodynamic equlibrium. It was originally presented in >>refer H- test Ferland, G. J., & Persson, S. E. 1989, ApJ, 347, 656

---

limit_lte_metal.in

STE with metals

```
title STE with metals
# this tests whether thermal processes go to STE
#
# commands controlling continuum =========
# a dilution factor of 1 is one way to get STE
black body, t = 20000 dilution 1
#
# commands for density & abundances =========
```

```
hden 10
abundances starburst 5
#
# commands controlling geometry =========
stop zone 1
stop lyman optical depth -6
set dr -10
#
# other commands for details =========
iterate
#
# commands controlling output =========
print departure coef element hydrogen
print populations h-like hydrogen
save overview "limit_lte_metal.ovr"
save performance "limit_lte_metal.per"
save heating "limit_lte_metal.het" last
save cooling "limit_lte_metal.col" last
#
# limit_lte_metal.in
# class limit
# ======================================
#
```

This checks that the code goes to strict thermodynamic equilibrium for the case of a metal rich gas exposed to a true black body. The many heavy element lines should dominate cooling, so this is a test that the multilevel atoms go to LTE in the radiation-dominated limit.

Checks:
- Temperature should equilibrate at 20000 K.
- Departure coefficients should equal unity.

`limit_recoil_ion.in`

test compton recoil ionization of hydrogen

```
title test compton recoil ionization of hydrogen
#
# commands controlling continuum =========
laser 2000 ryd
ionization parameter -5
#
# commands for density & abundances =========
hden 0
init "honly.ini"
#
# commands controlling geometry =========
set dr 14
stop zone 10
#
# other commands for details =========
iterate
no secondary ionization
constant temperature 1000
#
# commands controlling output =========
save overview "limit_recoil_ion.ovr"
save performance "limit_recoil_ion.per"
#
#
# limit_recoil_ion.in
# class limit
```

```
# ======================================
#
```

H ionization is totally due to recoil ionization in this model. The assert checks the final hydrogen ionization.

`limit_strom.in`

pure-H Stromgren sphere

```
title pure-H Stromgren sphere
# the answer is R(Stromgren) = 4.16E17 cm
#
# commands controlling continuum =========
blackbody 50000 K
q(h) 49
#
# commands for density & abundances =========
hden 4
init file "honly.ini"
abundances all -10
#
# commands controlling geometry =========
sphere static
radius 16
stop efrac -0.5
#
# other commands for details =========
no level2
turbulence 20 km/s
constant temper 7500
iterate
#
# commands controlling output =========
save performance "limit_strom.per"
save overview last "limit_strom.ovr"
save results last "limit_strom.rlt"
save dr last "limit_strom.dr"
#
# limit_strom.in
# class limit
# ======================================
#
```

This case checks that the code computes the geometry and emissivity correctly for a pure hydrogen spherical shell. The low temperature is chosen to avoid collisional ionization. The model stops at the Ho-H+ ionization front. The turbulence is to prevent the Balmer lines from becoming optically thick.
Checks
- Outer radius should be 4.16391017 cm.
- Predicted Hb, case B Hb, and Q(H) Hb, all agree.

`limit_supra.in`

secondary ionization dominated gas

```
title secondary ionization dominated gas
# like SN envelope
#
# commands controlling continuum =========
# this continuum will be VERY faint
table agn
```

```
ionization parameter -25
# secondary ioinzations will dominate
set csupra -5
#
# commands for density & abundances =========
hden 5
abundances old solar 84
#
# commands controlling geometry =========
stop temperature 20
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 1000 K
iterate convergence
#
# commands controlling output =========
print ages
save overview "limit_supra.ovr"
save performance "limit_supra.per"
save heating "limit_supra.het"
save ionizing continuum "limit_supra.ion" last
save molecules "limit_supra.mol"
#
#
# limit_supra.in
# class limit
# ======================================
#
```

This model computes the ionization within cool gas that is totally ionized by suprathermal secondary electrons.

Charge transfer heating is VERY important in this simulation.

`limit_thick_brems.in`

optically thick brems

```
title optically thick brems
#
# check that optically thick brems emission approaches the RJ limit
#
# commands controlling continuum =========
blackbody 2e5
#
# we need to test this command in at least one sim
Xi 3
#
# commands for density & abundances =========
hden 6
#
# commands controlling geometry =========
stop column density 20
#
# other commands for details =========
constant temperature 1e4
iterate 3
set nFnu diffuse outward
set nFnu add 2e-8 ryd
set nFnu add 5e-8 ryd
set nFnu add 1e-7 ryd
set nFnu add 2e-7 ryd
set nFnu add 5e-7 ryd
set nFnu add 1e-6 ryd
```

```
set nFnu add 2e-6 ryd
set nFnu add 5e-6 ryd
set nFnu add 1e-5 ryd
set nFnu add 2e-5 ryd
set nFnu add 5e-5 ryd
#
# commands controlling output =========
print line faint -10
save continuum "limit_thick_brems.con" last units microns
save optical depth "limit_thick_brems.opd" last
save overview "limit_thick_brems.ovr"
save dr "limit_thick_brems.dr"
#
# commands giving the asserts =========
#
#
# limit_thick_brems.in
# class limit
# ======================================
#
```

At some point we had a major bug affecting the optically thick part of the radio free-free emission. This sim checks that the optically thick emission from a plane-parallel slab has the correct Rayleigh-Jeans shape. This implies that at long wavelengths nuFnu should vary as lambda^3.

`limit_vbhum.in`

compare with Van Blerkom and Hummer exact RT results

```
title compare with Van Blerkom and Hummer exact RT results
#
# commands controlling continuum =========
blackbody 50000 K
phi(h) 12.30103
# commands for density & abundances =========
hden 4
init "honly.ini"
abundances all -10
#
# commands controlling geometry =========
stop efrac -0.5
#
# other commands for details =========
diffuse ots
no level2 lines
constant temper 4
iterate
#
# commands controlling output =========
save performance "limit_vbhum.per"
save overview last "limit_vbhum.ovr"
save dr last "limit_vbhum.dr"
#
#
# limit_vbhum.in
#
# class limit
# ======================================
#
```

This is a test of the treatment of the diffuse fields, their transfer, and their effects on the ionization structure of a nebula. The comparison is made against the exact calculation published by Van Blerkom and Hummer (1967). The geometry is open, that is, similar to that assumed in most BLR calculations.

>>refer H ionization Van Blerkom, D., & Hummer, D. G. 1967, MNRAS, 137, 353

The diffuse ots command is entered in order to reproduce the Van Blerkom and Hummer results. The default assumption, outward only, does not agree as well. I changed the default from OTS to outward only to be in better agreement with predictions by Harrington and Rubin at the Lexington meeting. They have not checked whether their codes are in agreement with the Van Blerkom and Hummer paper.

Checks:
- Neutral fraction at illuminated face 5.8*10-4.
- Location of ionization front at 7.8*1016 cm.
- 34He 1 486134 and 34CA B 486134 agree; both slightly lower than 34Q(H) 486134.
- Answers with OTS agree with 1967 results.

test hydrogen ground state rec effic against vb+h exact results this is their case e) - "zero condition" their answer for H0/Htot at the illuminated edge is approx 5.8E-4, and a Stromgren radius of approximately 7.7E16 cm

---

`limit_veryveryfast.in`

very fast simulation for Purify/valgrind

```
title very fast simulation for Purify/valgrind
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
no file opacity
set dr 0
#
# commands for density & abundances =========
hden 9
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no level 2
constant temperature 4
database h-like levels small
database he-like levels small
#
# commands controlling output =========
save overview "limit_veryveryfast.ovr"
save performance "limit_veryveryfast.per"
save dr last "limit_veryveryfast.dr"
#
#
# limit_veryveryfast
# class limit
# ======================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

`lya-21cm-constant.in`

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm constant
#
# commands controlling output =========
#
set save prefix "lya-21cm-constant"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu=constant case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

`lya-21cm-excitation.in`

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
```

```
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm excitation
#
# commands controlling output =========
#
set save prefix "lya-21cm-excitation"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu~B(Texc) case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

`lya-21cm-kinetic.in`

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm kinetic
```

```
#
# commands controlling output =========
#
set save prefix "lya-21cm-kinetic"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu~B(Tkin) case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

`nlr_lex00.in`

NLR model for Lexington 2000 Meeting

```
title NLR model for Lexington 2000 Meeting
#
# commands controlling continuum =========
phi(h) 12.47712
# shape of continuum is interpolated table
interpolate (0 -10) (0.08 -10) (0.1 1) (3676 -4.935) (4700 -11)
continue (4750 -20) (7.4e6 -30)
#
# commands controlling geometry =========
stop column 22
#
# commands for density & abundances =========
hden 4
init file="c84.ini"
abundances He=-1 c=-3.52 n=-4 o=-3.097 ne=-4 na=-9
continue mg=-4.523 al=-8 si=-4.523 s=-4.824 ar=-9 ca=-8 fe=-8 ni=-9
#
# other commands for details =========
iterate
#
# commands controlling output =========
print line faint .01
# add sum of these lines to printout for Stoy ratio
print line sum
H 1 1215.67A
Blnd 5875.66A
blnd 1909
blnd 1549
N 2 6583.45
N 2 6548.05
n 3 57.3238m
blnd 1750
blnd 1486
O 1 6300.30
o 1 63.1679m
blnd 3727
blnd 1666
O 3 51.8004m
o 3 5006.84
o 3 4958.91
blnd 1402
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
```

```
Blnd 2424
Ne 5 3425.88A
Ne 5 3345.82A
blnd 2798
si 2 34.8046m
Blnd 6720
S 3 18.7078m
S 3 9530.62
S 3 9068.62
S 4 10.5076m
end of lines
#
save performance "nlr_lex00.per"
save overview last "nlr_lex00.ovr"
save dr last "nlr_lex00.dr"
save results last "nlr_lex00.rlt"
#
# nlr_lex00.in
# class nlr
# ======================================
```

This is one of the test cases from the Lexington (1993) Meeting suite of nebulae. It is a grain-free NLR model.

`nlr_liner.in`

NLR liner model

```
title NLR liner model
# a constant pressure (gas+radiation) model of a nlr_liner cloud
# in the spirit of Ferland and Netzer 1983
#
# commands controlling continuum =========
table agn
ionization parameter -3
#
# commands for density & abundances =========
hden 6
init file "ism.ini"
abundances old solar 84
metals 0.3
#
# commands controlling geometry =========
stop thickness 16.3
stop column density 23
constant pressure
#
# other commands for details =========
#
# commands controlling output =========
save performance "nlr_liner.per"
save overview last "nlr_liner.ovr"
save element nitrogen last "nlr_liner.nit"
save dr last "nlr_liner.dr"
save results last "nlr_liner.rlt"
#
# nlr_liner.in
# class nlr
# ======================================
```

This is a model somewhat like the Liner parameters proposed by Ferland and Netzer (1983). A second iteration is performed to allow the calculation of the line radiation pressure.

>>refer nlr_liner model Ferland, G. J., & Netzer, H. 1983, ApJ, 264, 105

---

nlr_liner_grains.in

liner model with grains

```
title liner model with grains
#
# a constant pressure (gas+radiation) model of a liner cloud
# in the spirit of Ferland and Netzer 1983
#
# commands controlling continuum =========
ionization parameter -3
table agn
#
# commands for density & abundances =========
hden 6
# this turns on both grains and depleted abundances
abundances ism no grains
grains ism no qheat single
init file "ism.ini"
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
constant pressure
#
# commands controlling output =========
save performance "nlr_liner_grains.per"
save overview last "nlr_liner_grains.ovr"
save dr last "nlr_liner_grains.dr"
save continuum last "nlr_liner_grains.con" units microns
save results last "nlr_liner_grains.rlt"
#
# nlr_liner_grains.in
# class nlr
# ========================================
#
```

This is a model somewhat like the Liner parameters proposed by Ferland and Netzer (1983). A second iteration is performed to allow the calculation of the line radiation pressure. It includes grains and is so more realistic.

>>refer liner model Ferland, G. J., & Netzer, H. 1983, ApJ, 264, 105

---

nlr_paris.in

Paris meeting NLR model

```
title Paris meeting NLR model
#
# commands controlling continuum =========
interpolate (0 -10) (0.073 -10) (0.074 1) (7352 -4)
continue (7400 -15) (7.353e6 -20)
ionization parameter -2
#
# commands controlling geometry =========
stop lyman continuum optical depth 4
#
# commands for density & abundances =========
hden 3
init file="c84.ini"
abund He=-1 C=-3.5229 N=-4. O=-3.22185 ne=-3.82391 na=-8 mg=-4.5229 al=-8
continue si=-4.5229 s=-4.82391 ar=-8 ca=-8 fe=-7 ni=-8
```

```
#
# other commands for details =========
# this large group of lines are turned off so that the model runs
# 30 percent faster - lines are mainly fuv and x-ray, which we will
# not track in this model
no level2
iterate
database h-like element helium levels resolved 10
#
# commands controlling output =========
save performance "nlr_paris.per"
save overview last "nlr_paris.ovr"
save dr last "nlr_paris.dr"
save results last "nlr_paris.rlt"
#
# nlr_paris.in
# class nlr
# ======================================
```

This is the NLR model presented in the Meudon meeting on model nebulae. The init file is entered to make the code behave more like version 84.

Checks:
- init file works

`nova_dqher.in`

cold nova shell

```
title cold nova shell
# Ferland et al. 1984 DQ Her
# model of room temperature ionized cloud arund old nova DQ Her
# roughly that of
# tests behaviour of code at very low temperatures
#
# commands controlling continuum =========
# flat continuum, followed by nu^-2 power law
interpolate (0 0) (0.3 0) (8.e6 -14.8)
luminosity total 34
#
# commands for density & abundances =========
hden = 2.
abundances nova
grains no qheat single
#
# commands controlling geometry =========
filling factor 0.667
covering factor 0.667
radius 16.5682 , thickness = 16.14613
# need this since gas is so cool
stop temp = 100
#
# other commands for details =========
cosmic rays background
iterate
turbulence 300
database h-like element hydrogen levels resolved 15
database h-like element helium levels resolved 15
#
# commands controlling output =========
normalize to label="CaBo" 4861.32A intensity 1.169
print line all
# the normalizing line is not defined on the emergent line stack
print lines emergent off
```

```
save performance "nova_dqher.per"
save overview last "nova_dqher.ovr"
save results last "nova_dqher.rlt"
save dr last "nova_dqher.dr"
save transmitted continuum "nova_dqher.trn" last
#
# nova_dqher.in
# class nova
# ======================================
#
```

This tests the code39s behavior in the limit posed by the metal rich low density nebula surrounding DQ Her (Ferland et al. 1984).
Checks:
- Thickness exact
- Thermal stability High-Z gas ionization at low temperature

`nova_photos.in`

dense nova photosphere

```
title dense nova photosphere
set save prefix "nova_photos"
#
# commands controlling continuum =========
# this is the result of this command
# table star kurucz 35000; use old atlas atmosphere
# and makes it possible to run sims without
# installing the stellar atmosphere files
# set SED of central star
table SED "star_kurucz_35000.dat"
# set luminosity of central star
absolute bolometric magnitude -8.1
#
# commands for density & abundances =========
#
# commands controlling geometry =========
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint -1
save performance ".per"
save overview ".ovr" last
save convergence reason ".cvg" no hash
save results ".rlt" last
save dr ".dr" last
save heat ".het" last
save cool ".col" last
#
# nova_photos.in
# class nova
# ======================================
#
```

this model is intensely affected by continuum pumping of atoms. The hydrogen ionizaiton is by lyman line pumping, followed by photoionization from excited states.

`optimize_phymir.in`

test phymir optimizers

```
title test phymir optimizers
# spectrum computed with hden 5, temp 4
# subplex, phymir, powell
#
# commands controlling continuum =========
black 40000 K
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir
optimize iteration 100
# the following spectrum was derived by running this sim at hden 5 and t=4
# resulting eden was 5.039 and T=4, which we shall assert that we find
# >>chng 06 apr 03, backdate to old [OII] As and rederive spectrum
optimize lines
O 2 3728.81 0.1567
O 2 3726.03 0.4087
Blnd 7323 0.4344
Blnd 7332 0.3577
O 3 5006.84 3.8117
O 3 4363.21 0.0368
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "optimize_phymir.ovr"
save performance "optimize_phymir.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer can recover a known solution. The line spectrum was calculated at T = 1e4 K and and n_H=1e5 cm^-3, and resulted in the given electron density. The model optimize_subplex.in is a copy of this file.

`optimize_subplex.in`

test subplex optimizer

```
title test subplex optimizer
# spectrum computed with hden 5, temp 4
# subplex, phymir, amoeba, powell
#
# commands controlling continuum =========
black 40000 K
ionization par -3
#
# commands for density & abundances =========
```

```
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
constant temper 4.3 vary
optimize subplex
optimize iteration 100
optimize tolerance 0.01
# the following spectrum was derived by running this sim at hden 5 and t=4
# resulting eden was 5.039 and T=4, which we shall assert that we find
# >>chng 06 apr 03, backdate to old [OII] As and rederive spectrum
optimize lines
O 2 3728.81 0.1567
O 2 3726.03 0.4087
Blnd 7323 0.4344
Blnd 7332 0.3577
O 3 5006.84 3.8117
O 3 4363.21 0.0368
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "optimize_subplex.ovr"
save performance "optimize_subplex.per"
#
# optimize_subplex.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer can recover a known solution. The line spectrum was calculated at T = 1e4 K and and n_H=1e5 cm^-3, and resulted in the given electron density. The model optimize_phymir.in is a copy of this file.

`orion_hii_open.in`

conditions similar to Orion nebula blister

```
title conditions similar to Orion nebula blister
# orion hii region with open geometry
#
# commands controlling continuum =========
# SED of central star
table SED "star_kurucz_39600.dat"
# its flux of H-ionizing photons
phi(h) 13.0
#
# this is to include velocity field in radiative transfer
turbulence 8 km/sec no pressure
#
# commands for density & abundances =========
hden 4
abundances hii region no grains
grains orion
#
# commands controlling geometry =========
cosmic rays, background
constant pressure
# this is the account for continued matter beyond i front
double optical depths
```

```
#
# other commands for details =========
iterate 2
#
# commands controlling output =========
print line faint -5
# print lines as surface brightness
print lines surface brightness arcsec
print line optical depths
# want to print line intensities are surface brightness, per arcsec^2
print lines surface brightness arcsec
save pressure "orion_hii_open.pre"
save performance "orion_hii_open.per"
save overview last "orion_hii_open.ovr"
save dr last "orion_hii_open.dr"
save continuum last "orion_hii_open.con" units microns
save transmitted continuum last "orion_hii_open.trn"
save overview last "orion_hii_open.ovr"
save fine opacity last "orion_hii_open.opc" range 0.7 0.9 ryd
save element nitrogen last no hash "orion_hii_open.nit"
save lines, array "orion_hii_open.lina" units microns last no hash
save line emissivity "orion_hii_open.ems" last no hash emergent
H 1 4861.32A
O 3 5006.84A
Blnd 5199A
O 1 6300.30A
O 1 63.1679m
end of lines
save linelist "orion_hii_open.lin" "LineList_HII.dat" last no hash emergent absolute
#
# orion_hii_open.in
# class hii
# ======================================
```

This is a model similar in spirit to the blister geometry HII region model computed by Baldwin et al. (1991). Size-resolved Orion grains are included. The constant pressure command does a hydrostatic equilibrium structure. The predicted emission-line spectrum is affected by the reddening of the internal grains. The resulting t2 analysis produces artificial results as a result. This has an open geometry, the original BFM paper was a closed geometry. (This makes little difference). Background cosmic rays are also included although these should have little effect on warm ionized gas. The emission line spectrum is given in surface brightness units, as in the BFM paper.

`orion_hii_pdr.in`

constant pressure H+ region/pdr

```
title constant pressure H+ region/pdr
#
# commands controlling continuum =========
# the incident continuum is two parts
# star and flux of photons striking it
# this is the photosphere of the OVI star, its temperature and Q(H)
# this is the result of this command
# table star kurucz 39600 K
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_kurucz_39600.dat"
Q(H) 49
# this adds the observed hot brems, its temperature and the flux of
# photons striking the cloud
brems 6
phi(h) 10
# add cosmic rays, which are important in the pdr
cosmic rays, background
#
```

```
# commands controlling geometry =========
# this sets the separation from the star and the face of the cloud
radius 17.4507
# this turns off the stop temperature opption
# the sim will not stop due to temperature
stop temperature off
# this is typical of a gmc, larson 1981
stop total hydrogen column density 23
# this sets the thickness of the HII region & PDR
stop thickness 0.5 linear parsec
# constant total pressure, so like orion_hii_open
constant pressure
# this will result in a milli gauss B-field in molecular region
magnetic field -5 gauss
# the orion environment full covers the star, so turn on sphere
sphere
# we have a spherical geometry but want to simulate observing
# through a spectrometer's slit. use the aperture
# command for this
aperture beam
#
# other commands for details =========
# mimic existence of unmodeled molecular gas
double
# iterate since lines optically thick
iterate
# the observed microturbulence, partially a flow, so not included in pressure
turbulence 8 km/sec no pressure
# set the line width so lines appear on the save continuum
set save line width 10 km/s
# there should be no failures at all
failures 3
#
# commands for density & abundances =========
# this is the log of the initial H density, cm-3
hden 4
# this will speed up the calculation a bit
init file="ism.ini"
# this uses HII region abundances, but no grains
abundances hii region no grains
# this turns on orion grains, but leaves quantum heating off to save time
grains orion no qheat
# turn on PAHs, with an abundance that depends on H0 fraction,
# as suggested by long-slit observations of Orion bar,
# with an abundance 3x larger than default built into the code
grains PAH function 3
#
# commands controlling output =========
normalize to "O 1" 63.1679m
# print lots of faint CO lines
print line faint -4
save performance "orion_hii_pdr.per"
save overview last "orion_hii_pdr.ovr"
save heating "orion_hii_pdr.het"
save cooling "orion_hii_pdr.col"
save dr last "orion_hii_pdr.dr"
save results last "orion_hii_pdr.rlt"
save lines, array "orion_hii_pdr.lina" last, units microns
save continuum last "orion_hii_pdr.con" units microns
save hydrogen 21 cm last "orion_hii_pdr.21cm"
save hydrogen lya last "orion_hii_pdr.lya"
save element silicon last "orion_hii_pdr.sil"
save grain extinction last "orion_hii_pdr.grnext"
save grain charge last "orion_hii_pdr.grnchr"
save grain potential last "orion_hii_pdr.grnpot"
save grain temperature last "orion_hii_pdr.grntem"
#
#
#
# orion_hii_pdr.in
```

```
# class hii pdr
# ======================================
```

This extends BFM from the H+ region into the PDR as in Abel et al 2005. This is the correct way to do a PDR calcualtion.

>>refer Orion model Baldwin, J., Ferland, G. J., >>refercon Martin, P. G., Corbin, M., Cota, S., Peterson, >>refercon B. M., & Slettebak, A. 1991, ApJ, 374, 580

>>refer physics HII/PDR Abel, N.P., Ferland, G.J., Shaw, G. & >>refercon van Hoof, P.A.M. 2005, ApJS, 161, 65

`orion_hii_pdr_fast.in`

constant gas pressure H+ region/PDR

```
title constant gas pressure H+ region/PDR
# much faster due to physics disabled by fast.ini
#
# commands controlling continuum =========
# the incident continuum is two parts
# star and flux of photons striking it
# this is the result of this command
# table star kurucz 39600 K
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_kurucz_39600.dat"
Q(H) 49
# add cosmic rays, which are important at depth
cosmic rays, background
# plus hot brems
brems 6
phi(h) 10
#
# commands for density & abundances =========
hden 4
init file="fast.ini"
abundances hii region no grains
# single sized grain with no quantum heating
grains orion no qheat single
#
# commands controlling geometry =========
radius 17.4507
sphere
# let it go into the molecular cloud
stop temperature 10 linear
# this is roughly the thickness of OMC1
stop thickness 1 linear parsec
# mimic existence of unmodeled molecular gas with double command
double
#
# other commands for details =========
failures 3
iterate
# make constant gas pressure since fast turned off line radiation pressure
constant gas pressure
# the observed microturbulence
turbulence 8 km/sec
# we have a spherical geometry but want to simulate observing
# through a spectrometer's slit. use the aperture
# command for this
aperture beam
#
# commands controlling output =========
normalize to "CaBo" 4861.32A
print line faint -4
# the normalizing line is not defined on the emergent line stack
```

```
print lines emergent off
save performance "orion_hii_pdr_fast.per"
save overview last "orion_hii_pdr_fast.ovr"
save heating "orion_hii_pdr_fast.het"
save cooling "orion_hii_pdr_fast.col"
save dr last "orion_hii_pdr_fast.dr"
save results last "orion_hii_pdr_fast.rlt"
save continuum last "orion_hii_pdr_fast.con" units microns
save ionizing continuum last "orion_hii_pdr_fast.ion"
save hydrogen 21 cm last "orion_hii_pdr_fast.21cm"
save hydrogen lya last "orion_hii_pdr_fast.lya"
save element silicon last "orion_hii_pdr_fast.sil"
save element sulphur last "orion_hii_pdr_fast.sul"
#
#
# orion_hii_pdr_fast.in
# class hii pdr
# ======================================
#
```

Orion HII region and PDR, simialr to orion_hii_pdr but much faster because of fast.ini

---

pdr_co_fully.in

H2 and CO in fully molecular limit

```
title H2 and CO in fully molecular limit
# this is a pair with pdr_co_fully_noneq - that tests non equilibrium chem
#
# commands controlling continuum =========
blackbody 5000
luminosity total solar linear 2
brems 6
luminosity total solar log -2.7
#
# commands for density & abundances =========
# set the density and composition, ism with grains
hden 10
abundances ism no qheat
#
# other commands for details =========
# this is an important ionization source
cosmic ray background
# code will stop at 4000 K by default, lower this temp so we
# can do fully molecular gas
stop temperature 10K linear
#
# commands controlling geometry =========
# the radius and thickness
radius 15.8
stop thickness 6
turbulence 3 km / s
#
# commands controlling output =========
save performance "pdr_co_fully.per"
save overview "pdr_co_fully.ovr"
save molecules "pdr_co_fully.mol"
save dr "pdr_co_fully.dr"
save heating "pdr_co_fully.het"
save cooling "pdr_co_fully.col"
save grain charge "pdr_co_fully.grnchr"
save grain drift "pdr_co_fully.grndft"
save grain temperature "pdr_co_fully.grntem"
save ionization means "pdr_co_fully.ion"
#
```

```
#
# gas has more he++ than He+ due to fast charge transfer with co
# neutralizing he+
# pdr_co_fully.in
# class pdr
# ======================================
```

test code in fully molecular limit this is a pair with pdr_co_fully_noneq - that tests non equilibrium chem

---

pdr_co_fully_noneq.in

H2 and CO are fully molecular, non-equilibrium case

```
title H2 and CO are fully molecular, non-equilibrium case
# this is a pair with pdr_co_fully.in, which does not include non-equil chem
#
# commands controlling continuum =========
blackbody 5000
luminosity total solar linear 2
brems 6
luminosity total solar log -2.7
#
# commands for density & abundances =========
# set the density and composition, ism with grains
hden 10
abundances ism no qheat
#
# other commands for details =========
# this is an important ionization source
cosmic ray background
# code will stop at 4000 K by default, lower this temp so we
# can do fully molecular gas
stop temperature 10K linear
#
# commands controlling geometry =========
# the radius and thickness
radius 15.8
stop thickness 6
turbulence 3 km / s
# this turns on non-equilibrium chemistry as suggested by Federman et al. 1996
set chemistry non equilibrium
#
# commands controlling output =========
save performance "pdr_co_fully_noneq.per"
save overview "pdr_co_fully_noneq.ovr"
save molecules "pdr_co_fully_noneq.mol"
save dr "pdr_co_fully_noneq.dr"
save heating "pdr_co_fully_noneq.het"
save cooling "pdr_co_fully_noneq.col"
save grain charge "pdr_co_fully_noneq.grnchr"
save grain drift "pdr_co_fully_noneq.grndft"
save grain temperature "pdr_co_fully_noneq.grntem"
#
#
# gas has more he++ than He+ due to fast charge transfer with co
# neutralizing he+
# pdr_co_fully_noneq.in
# class pdr
# ======================================
```

test code in fully molecular limit with Federman non-equilibrium chem this is a pair with pdr_co_fully.in, which does not include non-equil chem

---

pdr_coolbb.in

illumination by cool STE blackbody

```
title illumination by cool STE blackbody
# gasis fully molecular, grains should be in STE
#
# commands controlling continuum =========
# illuminate with 120 blackbody in thermodynamic equilibrium
blackbody 120 STE
CMB
#
# commands for density & abundances =========
# density
hden 7
# ism dust and grains
abundances ISM no grains
# dust to gas ratio is 10x standard
grains 1.0
# lowers metals and grains to 1/10 standard, so metals are
# 1/10 solar while dust to gas ratio is galactic
metals and grains 0.1
#
# other commands for details =========
# CO heating sets dr on second iteration, need many zones
set nend 1600
# set background cosmic rays to allow chemistry
cosmic ray background
# we need iterate to convergence here, but that doesn't work for now...
iterate convergence
#
# commands controlling geometry =========
radius 17.5
sphere
stop temperature 20K linear
stop column density 25.5
# double optical depths in PDR sims, to account for unmodelled
# molecular cloud behind the PDR
double
#
# commands controlling output =========
save performance "pdr_coolbb.per"
save overview "pdr_coolbb.ovr"
save heating "pdr_coolbb.het"
save cooling "pdr_coolbb.col"
save dr "pdr_coolbb.dr"
save grain temperature "pdr_coolbb.grntem"
save convergence reason "pdr_coolbb.cvr"
save lines emissivity "pdr_coolbb.ems"
H2O 212.468m
H2O 160.466m
CO 325.137m
CO 144.745m
CO 118.548m
CN 880.858m
end
#
#
# pdr_coolbb.in
# class pdr
# ======================================
```

This is a dense ISM exposed to a cool blackbody. This tests the ability to converge onto a VERY molecular environment. Nearly all C and H are in CO and H2. Cosmic rays are the main source of heat and ionization.

Continuum pumping of CO followed by collisional deexcitation is a major heating agent across the sim.

pdr_dense_persei.in

dense phase zeta persei cloud

```
title dense phase zeta persei cloud
#
# density and abundances ==========
# density of dense phase from Table 2 of Le Petit paper ========
hden 4.3
#
# abundandces from Table 1 of Le Petit paper ==========
element carbon abundance 0.000132 linear
element helium abundance 0.10 linear
element oxygen abundance 0.00032 linear
element nitrogen abundance 0.000075 linear
element sulphur abundance 0.0000186 linear
element silicon abundance 0.000029 linear
# set abundance of all other elements to zero ====================
element copper off
element magnesium off
element manganese off
element sodium off
element chlorine off
element vanadium off
element potassium off
element phosphorous off
element calcium off
element iron off
element zinc off
element neon off
element argon off
element fluorine off
element aluminum off
element boron off
element lithium off
element beryllium off
element scandium off
element nickel off
element titanium off
element chromium off
element cobalt off
# do not use Federman rates for this model ==============
set federman chemistry off
# use standard ism grain size distribution ============
grains ism
#
# command controlling the continuum, for this model is Draine 1978 field ====
table draine 0.5 linear
# make sure no H-ioinizing radiation strikes the cloud
extinguish 24
#
# fix the temperature to 20 K =============
constant temperature 20
# stop at a radius of 4.3e-4 parsecs ============
stop thickness 0.00043 parsecs linear
# Le Petit model does not consider ices, so turn this off ============
no grain molecules
# turn on cosmic rays =========
cosmic rays background
# Set cosmic ray ionization rate to Table 2 of Le Petit paper ========
set csupra -15.6
# Allow calculation to go extend into cold environment ============
stop temperature linear 3
#
# commands controlling output ============
save performance "pdr_dense_persei.per"
```

```
save overview "pdr_dense_persei.ovr"
save dr "pdr_dense_persei.dr"
save molecules "pdr_dense_persei.mol"
save heating "pdr_dense_persei.het"
save cooling "pdr_dense_persei.col"
#
# pdr_dense_persei.in
# class pdr
# ===================================
```

This is the dense phase model presented by LePetit, Roueff, and Herbst in order to reproduce C2 and C3 column densities observed along the line of sight to zera persei. This is our attempt at reproducing their calculation. This is the dense molecular phase, not the phase that produces H3+

>>refer model pdr Le Petit, F., Roueff, E., & Herbst, E. 2004, # >>refercon A&A, 417, 993

If you do a thermal equilibrium calculation by removing the constant temperature command the kinetic temperature will be about three times larger than assumed in their paper.

---

pdr_HTT91.in

low-density PDR from HTT91

```
title low-density PDR from HTT91
# >>refer test model Hollenbach, D., Takahashi, T., &
# >>refcon Tielens, A.G.G.M., 1991, ApJ,377, 192-209
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
# this is hot star continuum
black 30000
intensity 0.2 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
cosmic rays, background
#
# commands for density & abundances =========
hden 3
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
grains orion, abundance log 0.16 no qheat
#
# commands controlling geometry =========
sphere
# stop when gas is fully neutral
stop efrac -10
# this is to stop at an intended place, since results would be
# very dependent on details if we stop on temperature
stop thickness 18.954
# stop when gas is cold
stop temperature 10 linear
# add this to mimic unmodelled neutral gas
double optical depths
#
# other commands for details =========
iterate 2
Database H-like Lyman pumping off
turbulence 1.5 km/sec
#
# commands controlling output =========
normalize to "C 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
```

```
print line pump
print line optical depths
print ages
save performance "pdr_HTT91.per"
save overview last "pdr_HTT91.ovr"
save dr "pdr_HTT91.dr"
save molecules last "pdr_HTT91.mol"
save results last "pdr_HTT91.rlt"
save continuum units microns last "pdr_HTT91.con"
save heating last "pdr_HTT91.het"
save cooling last "pdr_HTT91.col"
#
# pdr_HTT91.in
# class pdr
# ======================================
#
```

This is the Hollenbach et al 1991 Low-density PDR The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

there is very little CO in this model since it is not thick enough for the UV pumping lines to become optically thick

---

pdr_leiden_f1.in

Leiden meeting model 1

```
title Leiden meeting model 1
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
print line optical depths
save performance "pdr_leiden_f1.per"
save overview "pdr_leiden_f1.ovr"
save continuum "pdr_leiden_f1.con"
save leiden lines "pdr_leiden_f1.lin"
save leiden "pdr_leiden_f1.lei"
save dr "pdr_leiden_f1.dr"
save molecules "pdr_leiden_f1.mol"
save grain physical conditions "pdr_leiden_f1.grn"
save chemistry rates "pdr_leiden_f1.COr" "CO"
save chemistry rates "pdr_leiden_f1.H2r" "H2"
```

```
save chemistry rates "pdr_leiden_f1.H2a" "H2" all
save chemistry rates "pdr_leiden_f1.H2ds" "H2" destruction
save chemistry rates "pdr_leiden_f1.H2cr" "H2" creation
save chemistry rates "pdr_leiden_f1.H2ca" "H2" catalytic
save secondaries "pdr_leiden_f1.sec"
save species column densities "pdr_leiden_f1.col" all
#
#
#
# pdr_leiden_f1.in
# class pdr
# ========================================
#
```

This sim has some interesting properties. The grain temp is so low that O freezes onto grains as H2O. This is so efficient that CO does not become well formed - the CO/C ratio only reaches 0.3. This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f2.in

Leiden meeting model 2

```
title Leiden meeting model 2
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use
# half the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_f2.per"
save overview "pdr_leiden_f2.ovr"
save continuum "pdr_leiden_f2.con"
save molecules "pdr_leiden_f2.mol"
save chemistry rates "pdr_leiden_f2.rat" "SiO"
save leiden lines "pdr_leiden_f2.lin"
save leiden "pdr_leiden_f2.lei"
save dr "pdr_leiden_f2.dr"
save grain physical conditions "pdr_leiden_f2.grn"
#
#
# pdr_leiden_f2.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f3.in

Leiden meeting model 3

```
title Leiden meeting model 3
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_f3.per"
save overview "pdr_leiden_f3.ovr"
save continuum "pdr_leiden_f3.con"
save leiden lines "pdr_leiden_f3.lin"
save leiden "pdr_leiden_f3.lei"
save dr "pdr_leiden_f3.dr"
save grain physical conditions "pdr_leiden_f3.grn"
#
#
# pdr_leiden_f3.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f4.in

Leiden meeting model 4

```
title Leiden meeting model 4
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
#
# commands for density & abundances =========
grains ism 1.16 no qheat
#
```

```
# commands controlling geometry =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
# hydrogen density
hden 5.5
#
# commands controlling output =========
save performance "pdr_leiden_f4.per"
save overview "pdr_leiden_f4.ovr"
save continuum "pdr_leiden_f4.con"
save leiden lines "pdr_leiden_f4.lin"
save leiden "pdr_leiden_f4.lei"
save dr "pdr_leiden_f4.dr"
save grain physical conditions "pdr_leiden_f4.grn"
#
#
# pdr_leiden_f4.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

`pdr_leiden_hack_f1.in`

Leiden meeting model 1 with hacks

```
title Leiden meeting model 1 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
```

```
# commands controlling output =========
save performance "pdr_leiden_hack_f1.per"
save leiden lines "pdr_leiden_hack_f1.lin"
save leiden "pdr_leiden_hack_f1.lei"
save dr "pdr_leiden_hack_f1.dr"
save grain physical conditions "pdr_leiden_hack_f1.grn"
save overview "pdr_leiden_hack_f1.ovr"
#
#
#
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 this includes hacks to get "standard answer"

---

pdr_leiden_hack_f2.in

Leiden meeting model 2 with hacks

```
title Leiden meeting model 2 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use
# half the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_hack_f2.per"
save leiden lines "pdr_leiden_hack_f2.lin"
save leiden "pdr_leiden_hack_f2.lei"
save dr "pdr_leiden_hack_f2.dr"
save grain physical conditions "pdr_leiden_hack_f2.grn"
save overview "pdr_leiden_hack_f2.ovr"
#
#
# pdr_leiden_hack_f2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_f3.in

Leiden meeting model 3 with hacks

```
title Leiden meeting model 3 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_hack_f3.per"
save leiden lines "pdr_leiden_hack_f3.lin"
save overview "pdr_leiden_hack_f3.ovr"
save leiden "pdr_leiden_hack_f3.lei"
save dr "pdr_leiden_hack_f3.dr"
save grain physical conditions "pdr_leiden_hack_f3.grn"
#
#
# pdr_leiden_hack_f3.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 include hacks to get standard answer.

`pdr_leiden_hack_f4.in`

Leiden meeting model 4 with hacks

```
title Leiden meeting model 4 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
#
# commands for density & abundances =========
grains ism 1.16 no qheat
#
# commands controlling geometry =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
```

```
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
# hydrogen density
hden 5.5
#
# commands controlling output =========
save performance "pdr_leiden_hack_f4.per"
save leiden lines "pdr_leiden_hack_f4.lin"
save leiden "pdr_leiden_hack_f4.lei"
save dr "pdr_leiden_hack_f4.dr"
save grain physical conditions "pdr_leiden_hack_f4.grn"
save overview "pdr_leiden_hack_f4.ovr"
#
#
# pdr_leiden_hack_f4.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks needed to get standard answer.

`pdr_leiden_hack_v1.in`

Leiden meeting model 5 with hacks

```
title Leiden meeting model 5 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# is half the requested value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
#
# commands controlling output =========
save performance "pdr_leiden_hack_v1.per"
save leiden lines "pdr_leiden_hack_v1.lin"
save leiden "pdr_leiden_hack_v1.lei"
save dr "pdr_leiden_hack_v1.dr"
save grain temperature "pdr_leiden_hack_v1.grn"
save overview "pdr_leiden_hack_v1.ovr"
```

```
#
#
# pdr_leiden_hack_v1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_v2.in

Leiden meeting model 6 with hacks

```
title Leiden meeting model 6 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v2.per"
save leiden lines "pdr_leiden_hack_v2.lin"
save leiden "pdr_leiden_hack_v2.lei"
save dr "pdr_leiden_hack_v2.dr"
save grain temperature "pdr_leiden_hack_v2.grn"
save overview "pdr_leiden_hack_v2.ovr"
save heating "pdr_leiden_hack_v2.het"
save cooling "pdr_leiden_hack_v2.col"
save h2 rates "pdr_leiden_hack_v2.h2rat"
#
#
# pdr_leiden_hack_v2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_v3.in

Leiden meeting model 7 with hacks

```
title Leiden meeting model 7 with hacks
```

```
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# this sim has more than one thermal solution - force into lowest one,
# the one found by the rest of the group - without this we will find a
# soln at 1400 K
force temperature to 60K
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v3.per"
save leiden lines "pdr_leiden_hack_v3.lin"
save leiden "pdr_leiden_hack_v3.lei"
save dr "pdr_leiden_hack_v3.dr"
save grain temperature "pdr_leiden_hack_v3.grn"
save overview "pdr_leiden_hack_v3.ovr"
save heating "pdr_leiden_hack_v3.het"
save cooling "pdr_leiden_hack_v3.col"
#
#
# pdr_leiden_hack_v3.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer

---

`pdr_leiden_hack_v4.in`

Leiden meeting model 8 with hacks

```
title Leiden meeting model 8 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
```

```
set PAH Bakes
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v4.per"
save leiden lines "pdr_leiden_hack_v4.lin"
save leiden "pdr_leiden_hack_v4.lei"
save dr "pdr_leiden_hack_v4.dr"
save grain temperature "pdr_leiden_hack_v4.grn"
save overview "pdr_leiden_hack_v4.ovr"
save heating "pdr_leiden_hack_v4.het"
save cooling "pdr_leiden_hack_v4.col"
save transmitted continuum "pdr_leiden_hack_v4.con"
#
#
# pdr_leiden_hack_v4.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

`pdr_leiden_v1.in`

Leiden meeting model 5

```
title Leiden meeting model 5
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# is half the requested value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
# add PAHs
grains PAH no qheat 3 function
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v1.per"
save overview "pdr_leiden_v1.ovr"
save leiden lines "pdr_leiden_v1.lin"
save leiden "pdr_leiden_v1.lei"
save dr "pdr_leiden_v1.dr"
save grain temperature "pdr_leiden_v1.grn"
```

```
#
#
#
# pdr_leiden_v1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_v2.in

Leiden meeting model 6

```
title Leiden meeting model 6
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v2.per"
save overview "pdr_leiden_v2.ovr"
save leiden lines "pdr_leiden_v2.lin"
save leiden "pdr_leiden_v2.lei"
save dr "pdr_leiden_v2.dr"
save grain temperature "pdr_leiden_v2.grn"
#
#
# pdr_leiden_v2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_v3.in

Leiden meeting model 7

```
title Leiden meeting model 7
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
```

```
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v3.per"
save overview "pdr_leiden_v3.ovr"
save leiden lines "pdr_leiden_v3.lin"
save leiden "pdr_leiden_v3.lei"
save dr "pdr_leiden_v3.dr"
save grain temperature "pdr_leiden_v3.grn"
save heating "pdr_leiden_v3.het"
save cooling "pdr_leiden_v3.col"
#
#
# pdr_leiden_v3.in
# class pdr
# ======================================
#
```

---

pdr_leiden_v4.in

Leiden meeting model 8

```
title Leiden meeting model 8
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v4.per"
```

```
save overview "pdr_leiden_v4.ovr"
save leiden lines "pdr_leiden_v4.lin"
save leiden "pdr_leiden_v4.lei"
save dr "pdr_leiden_v4.dr"
save grain temperature "pdr_leiden_v4.grn"
save transmitted continuum "pdr_leiden_v4.con"
save heating "pdr_leiden_v4.het"
save cooling "pdr_leiden_v4.col"
#
#
# pdr_leiden_v4.in
# class pdr
# ======================================
#
```

---

pdr_minimal.in

test physical conditions at the illuminated face of a PDR

```
title test physical conditions at the illuminated face of a PDR
#
# commands controlling continuum =========
table draine 50000
extinguish 24
#
# commands for density & abundances =========
hden 5.5
element helium abundance -1.00
element lithium off
element beryllium off
element boron off
element carbon off
element oxygen off
element fluorine off
element neon off
element sodium off
element magnesium off
element aluminum off
element silicon off
element phosphorus off
element sulphur off
element chlorine off
element argon off
element potassium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element iron off
element cobalt off
element nickel off
element copper off
element zinc off
#
# other commands for details =========
constant temperature 50 linear
set dr 1
stop zone 2
stop temperature off
#
# commands controlling output =========
set save prefix "pdr_minimal"
save performance ".per" last
save overview ".ovr" last
```

```
save molecules ".mol" last
save leiden ".lei" last
save leiden lines ".lin" last
#
#
# IF EITHER OF THESE MONITORS NEEDS TO BE ADJUSTED, CHECK THAT THE IONIZATION
# CONDITIONS IN ZONE 1 AND 2 ARE IN VERY GOOD AGREEMENT!
#
# pdr_minimal.in
# class pdr
# ======================================
```

This model is derived from the F4 model from the Leiden workshop (Roellig et al. 2007, A&A, 467, 187). It has been reduced to a two-zone model in order to test the ionization conditions at the face of the PDR. Older versions of the code had a bug where the ionization in zone 1 was many dex lower than in zone 2. The conditions in zone 1 were wrong and should have been similar to the conditions in zone 2. Here we test that the code doesn't regress. See also ticket #358: https://wiki.nublado.org/ticket/358

The ionization in this sim is produced by continuum pumping of the metastable levels of N I, followed by photoionization out of the metastable levels of N I. See Ferland et al., 2012, ApJ, 757, 79. So this pumping and ionization mechanism is also tested by this sim.

`pdr_orion_veil.in`

Orion's veil

```
title Orion's veil
#
# commands controlling continuum =========
q(h) 50.000000
table SED "Rubin.sed"
# AGN & CMB background
background z=0
cosmic rays background
# as a test this was tried - atomic temperature raised fm 100 to 140
# but nothing really wrong
# the observed magnetic field, roughly 100 micro Gauss
magnetic field -4
#
# commands for density & abundances =========
hden 3.1
init "ism.ini"
element calcium on
abundances orion no grains
grains orion no qheat
element magnesium isotopes (24, 3) (25, 1) (26, 1)
#
# commands controlling geometry =========
stop neutral hydrogen column density 21.6
radius 19.1
stop temperature linear 5
# this will not be hit, but put it in to insure that we stop if
# gas becomes totally molecular
stop av 10
#
# other commands for details =========
failures 3
turbulence 0.5 km/sec
sphere
# c this simulates Lyman lines in the stellar continuum
# atom h-like lyman pumping off
#
# commands controlling output =========
print line optical depths
```

```
save overview "pdr_orion_veil.ovr"
save performance "pdr_orion_veil.per"
save PDR "pdr_orion_veil.pdr"
save species column densities "pdr_orion_veil.fe2col" "Fe+"
save hydrogen 21 cm "pdr_orion_veil.21cm"
save molecules "pdr_orion_veil.mol"
save overveiw "pdr_orion_veil.ovr"
save species column densities "pdr_orion_veil.cden" all
save heating "pdr_orion_veil.het"
save cooling "pdr_orion_veil.col"
save dr "pdr_orion_veil.dr"
save H2 rates "pdr_orion_veil.h2rat"
save pressure "pdr_orion_veil.pre"
save wind "pdr_orion_veil.wnd"
save continuum units microns "pdr_orion_veil.con" last
#
# pdr_orion_veil.in
# class pdr
# ======================================
#
```

This is Abel et al 2004 model of Orion's veil, the layer of gas in front of the Orion Nebula. >>refer Orion Veil Abel, N. P., Brogan, C. L., Ferland, G. J., >>refercon O'Dell, C. R., Shaw, G., & Troland, T. H. 2004

---

pdr_th85ism.in

TH85 PDR with ISM grains

```
title TH85 PDR with ISM grains
#
# commands controlling continuum =========
# cosmic radiation background
background z=0
# cosmic ray background ionization and heating
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
# their turbulence
turbulence 2.7 km/sec
# stopping criteria
# this should be the one actually used
stop AV 33.2 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness of 16.5 so that mole limit does not
# stop this calculation - that would make results very
# detail dependent
stop thickness 19
#
# commands for density & abundances =========
hden 5.362
# this turns off some elements, and processes we don't need
```

```
# so needs to come before the elements
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
# use ism abundances but turn of quantum heating
grains ism, abundance log 0.16 no qheat
#
# other commands for details =========
# must iterate since many FIR MIR lines are optically thick
iterate
# this is a closed geometry, in Orion, veil covers 2pi sr
sphere
# make Lyman lines very optically thick, which stops pumping by
# Balmer continuum
Database H-like Lyman pumping off
# this should run cleanly - turn down number of allow conv fails
failures 3
#
# commands controlling output =========
normalize to "c 2" 157.636m
# want the spectrum to be relative to this [C II] line
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "pdr_th85ism.per"
save overview last "pdr_th85ism.ovr"
save pdr last "pdr_th85ism.pdr"
save molecules last "pdr_th85ism.mol"
save dr last "pdr_th85ism.dr"
save hydrogen physical conditions last "pdr_th85ism.hyd"
save results last "pdr_th85ism.rlt"
save continuum units microns last "pdr_th85ism.con"
save heating last "pdr_th85ism.het"
save cooling last "pdr_th85ism.col"
save hydrogen 21 cm last "pdr_th85ism.21cm"
save element magnesium last "pdr_th85ism.mag"
save species levels "pdr_th85ism.lev" all
save species densities "pdr_th85ism.popCp" "C+[:]"
save species column density "pdr_th85ism.pop" "CO[:]"
save species densities "pdr_th85ism.poplist"
"*AV"
"*temp"
"e-"
C+
"C+[1:3]"
"CO[1]"
"CO[2]"
"H[1]"
"H[2]"
"He[1]"
"He[2]"
"He+[1]"
"He+[2]"
end of species
save grain extinction last "pdr_th85ism.grnext"
save grain potential last "pdr_th85ism.grnpot"
save grain temperature last "pdr_th85ism.grntem"
save grain charge last "pdr_th85ism.grnchr"
#
# pdr_th85ism.in
# class pdr
# ======================================
#
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR). Specifically, this is my attempt at their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

---

pdr_th85ism_cgto.in

TH85 pdr with ISM grains and C > O

```
title TH85 pdr with ISM grains and C > O
#
# commands controlling continuum =========
# cosmic radiation background
background z=0
# cosmic ray background ionization and heating
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
# their turbulence
turbulence 2.7 km/sec
# stopping criteria
# this should be the one actually used
stop AV 33.2 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness of 16.5 so that mole limit does not
# stop this calculation - that would make results very
# detail dependent
stop thickness 19
#
# commands for density & abundances =========
hden 5.362
# this turns off some elements, and processes we don't need
# so needs to come before the elements
init file="ism.ini"
# this is the TH85 mix except C is raised by 0.2 dex,
# and O lowered byt his amount, so that C/O > 1
abundances he= -1.01 c= -3.4 n=-8 o=-3.50 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
# use ism abundances but turn of quantum heating
grains ism, abundance log 0.16 no qheat
#
# other commands for details =========
# must iterate since many FIR MIR lines are optically thick
iterate
# this is a closed geometry, in Orion, veil covers 2pi sr
sphere
# make Lyman lines very optically thick, which stops pumping by
# Balmer continuum
Database H-like Lyman pumping off
# this should run cleanly - turn down number of allow conv fails
failures 3
#
# commands controlling output =========
```

```
normalize to "c 2" 157.636m
# want the spectrum to be relative to this [C II] line
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "pdr_th85ism_cgto.per"
save overview last "pdr_th85ism_cgto.ovr"
save pdr last "pdr_th85ism_cgto.pdr"
save molecules last "pdr_th85ism_cgto.mol"
save dr last "pdr_th85ism_cgto.dr"
save hydrogen physical conditions last "pdr_th85ism_cgto.hyd"
save results last "pdr_th85ism_cgto.rlt"
save continuum units microns last "pdr_th85ism_cgto.con"
save heating last "pdr_th85ism_cgto.het"
save cooling last "pdr_th85ism_cgto.col"
save hydrogen 21 cm last "pdr_th85ism_cgto.21cm"
save element magnesium last "pdr_th85ism_cgto.mag"
save grain extinction last "pdr_th85ism_cgto.grnext"
save grain potential last "pdr_th85ism_cgto.grnpot"
save grain temperature last "pdr_th85ism_cgto.grntem"
save grain charge last "pdr_th85ism_cgto.grnchr"
#
# pdr_th85ism_cgto.in
# class pdr
# ========================================
#
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR) but with the C abundance increased by 0.2 dex, and O lowered by this amount, so that C/O>1. Specifically, this is their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

`pdr_th85orion.in`

TH85 PDR with Orion grains

```
title TH85 PDR with Orion grains
#
# commands controlling continuum =========
# cosmic background
background
# galactic cosmic ray background
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands for density & abundances =========
hden 5.362
init file="ism.ini"
grains orion, abundance log 0.16 no qheat
abundances he=-1.01 c=-3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
```

```
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
sphere
# stopping criteria
# this should be the one actually used
# >>chn 04 mar 13, from 10 to 36.3, bug in AV had stopped at this depth,
# so change it to this to keep model the same
stop AV 36.3 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness so that would make results very
# detail dependent
stop thickness 19
#
# other commands for details =========
turbulence 2.7 km/sec
iterate
failures 3
#
# this is done to not allow pumping and subsequent photoionization
# of H by Balmer continuum in keeping with std pdr assumptions
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "c 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
#
save performance "pdr_th85orion.per"
save overview "pdr_th85orion.ovr"
save pdr last "pdr_th85orion.pdr"
# this only outputs major molecules
save molecules last "pdr_th85orion.mol"
save dr "pdr_th85orion.dr"
# this is to get all of H molecules
save hydrogen physical conditions last "pdr_th85orion.hyd"
save results last "pdr_th85orion.rlt"
save continuum units microns last "pdr_th85orion.con"
save ionizing continuum last "pdr_th85orion.ion"
save heating last "pdr_th85orion.het"
save cooling last "pdr_th85orion.col"
save hydrogen 21 cm last "pdr_th85orion.21cm"
# these are for the grains
save grain extinction last "pdr_th85orion.grnext"
save grain potential last "pdr_th85orion.grnpot"
save grain temperature last "pdr_th85orion.grntem"
save grain charge last "pdr_th85orion.grnchr"
#
#
# pdr_th85orion.in
# class pdr
# ======================================
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR). Specifically, this is my attempt at their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

pn_fluc.in

Paris PN with density fluctuations

```
title Paris PN with density fluctuations
set save prefix "pn_fluc"
#
# commands for density & abundances =========
fluctuations 16.5 4 3
# this sets up the code like version c84, with fewer chemical elements
init file="c84.ini"
# this sets the abundances of the elements that we will use
abund He=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 na=-10 mg=-4.523 al=-10
continue si=-4.523 s=-4.824 ar=-10 ca=-10 fe=-10 ni=-10
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
black 5
luminosity total 38
#
# commands controlling geometry =========
sphere
radius 17
#
# other commands for details =========
#
# commands controlling output =========
save performance ".per"
save overview last ".ovr"
save element nitrogen last ".nit"
save dr last ".dr"
save results last ".rlt"
#
# pn_fluc.in
# class pn function
# ========================================
```

The boundary conditions are similar to those for the Paris meeting PN, a homogeneous grain-free PN. This model has density fluctuations, with values chosen so that the mean ne np V are the same for the nebulae with and without fluctuations.

Checks:
- Check that the fluctuations command works.
- How do results compare with homogeneous Paris pn?

---

pn_ots.in

Paris PN with ots

```
title Paris PN with ots
# recompute "standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="c84.ini"
abund He=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 na=-10 mg=-4.523 al=-10
continue si=-4.523 s=-4.824 ar=-10 ca=-10 fe=-10 ni=-10
#
```

```
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
diffuse ots
no level2
iterate
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 15
#
# commands controlling output =========
save performance "pn_ots.per"
save overview last "pn_ots.ovr"
save element nitrogen last "pn_ots.nit"
save results last "pn_ots.rlt"
save dr last "pn_ots.dr"
#
# pn_ots.in
# class pn
# ======================================
#
```

This is the on-the-spot version of the Paris Planetary Nebula.
Checks:
- Q(H) total 4861 luminosity is close to expected value
- Line spectrum similar to that predicted by default conditions.

`pn_paris.in`

"Paris meeting PN"

```
title "Paris meeting PN"
set save prefix "pn_paris"
# standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="ism.ini"
# these elements were not part of the workshop models
element chlorine off
element argon off
element iron off
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 cl=-7 ar=-10 fe=-10
#
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
age 10^2^2 years
#
# commands controlling output =========
print lines sort wavelength
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line optical depths
print ages
print column densities
save performance ".per"
```

```
save overview ".ovr"
save transmitted continuum ".trn"
save continuum units microns ".con"
save element carbon ".car"
save physical conditions ".phy"
save element nitrogen ".nit"
save dr ".dr"
save temperature ".tem"
save lines emissivity ".ems"
h 1 6562.80A
Blnd 6720
end of lines
save averages ".avr" last
temperature hydrogen 1
end of averagers
#
# pn_paris.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations. A table in Hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes.

The model is meant to represent a planetary nebula ionized by a very hot central object. As a result there is a great deal of He++ and the associated line and continuum emission is very important.

An age of 10000 years was set. This tests logic in the age command.

---

pn_paris_cpre.in

"Paris meeting PN with constant pressure"

```
title "Paris meeting PN with constant pressure"
# standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
constant pressure
init file="ism.ini"
# these elements were not part of the workshop models
element chlorine off
element argon off
element iron off
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 cl=-7 ar=-10 fe=-10
#
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
age 10^2^2 years
#
# commands controlling output =========
print lines sort wavelength
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line optical depths
print ages
print column densities
```

```
save performance "pn_paris_cpre.per"
save overview "pn_paris_cpre.ovr"
save transmitted continuum "pn_paris_cpre.trn"
save continuum units microns "pn_paris_cpre.con"
save element carbon "pn_paris_cpre.car"
save physical conditions "pn_paris_cpre.phy"
save element nitrogen "pn_paris_cpre.nit"
save dr "pn_paris_cpre.dr"
save temperature "pn_paris_cpre.tem"
save lines emissivity "pn_paris_cpre.ems"
h 1 6562.80A
Blnd 6720
end of lines
save averages "pn_paris_cpre.avr" last
temperature hydrogen 1
end of averagers
#
# pn_paris_cpre.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations, modified by assuming constant pressure within the nebula.

`pn_paris_fast.in`

Paris PN, fast version

```
title Paris PN, fast version
# standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="fast.ini"
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 ar=-10
#
# commands controlling geometry =========
sphere
radius = 17
#
# other commands for details =========
#
# commands controlling output =========
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "pn_paris_fast.per"
save overview "pn_paris_fast.ovr"
save physical conditions "pn_paris_fast.phy"
save element nitrogen "pn_paris_fast.nit"
save dr "pn_paris_fast.dr"
#
# pn_paris_fast.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations. A table in Hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes.

The model is meant to represent a planetary nebula ionized by a very hot central object. As a result there is a great deal of He++ and the associated line and continuum emission is very important.

---

pn_sqrden.in

PN with density propt R^-2 and filling factor

```
title PN with density propt R^-2 and filling factor
# this is an optically thin model, which will have a broad range
# of density but the same ionization parameter across the model.
# the physical condtions should not vary by much across the structure
#
# commands controlling continuum =========
# continuum is hot blackbody at ~Ledd for solar mass
blackbody, t=5 luminosity=38
#
# commands for density & abundances =========
# the density will fall off as the inverse square of the radius, hence the name
hden 5 -2
init file "ism.ini"
# use default PN abundances but turn off quantum heating since
# we are not going to save the predicted near IR continuum
abundances planetary no qheat
#
# commands controlling geometry =========
# small filling factor so that region will be optically thin
filling factor -2
# set inner and outer radius
radius 16 18
sphere
#
# other commands for details =========
iterate
#
# commands controlling output =========
print line faint 1
save performance "pn_sqrden.per"
save overview "pn_sqrden.ovr" last
save dr "pn_sqrden.dr" last
save molecules "pn_sqrden.mol"
#
# pn_sqrden.in
# class pn
# ======================================
```

Checks:
- Zone thickness budgeting handled OK.
- physical conditions nearly constant across computed structure

---

rrc_o.in

he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3

```
title he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
#
# commands controlling continuum =========
laser 100
ionization -1
#
```

```
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element oxygen abundance -2.0458
element oxygen ionization -1 -1 -1 -1 -1 -1 -1 -1 -1
init file "ism.ini"
element helium off
element nitrogen off
element carbon off
element neon off
element magnesium off
element silicon off
element sulphur off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
constant temper 5
iterate
#
# commands controlling output =========
print line faint -5
save overview "rrc_o.ovr"
save performance "rrc_o.per"
save continuum "rrc_o.con" units Angstroms last
# rrc_o.in
# class limit
# ========================================
#
```

test RRC of simple and iso model atoms. The ionization is set to 10% for all stages of ionization of O. We monitor the ground state recombination emission. This is an optically thin model.

`stars_atlas.in`

Atlas stellar atmosphere

```
title Atlas stellar atmosphere
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star atlas 30400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
```

```
no blends
#
# commands controlling output =========
#
save performance "stars_atlas.per"
save overview last "stars_atlas.ovr"
save results last "stars_atlas.rlt"
save transmitted continuum last "stars_atlas.trn" no header
save continuum last "stars_atlas.con" units angstrom
#
# stars_atlas.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Atlas model atmosphere continua described by Kurucz (1991). Kevin Volk provided it as part of his original coding of these stellar atmosphere files. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

Checks: table star atlas command works.

`stars_atlas_3d.in`

Atlas stellar atmosphere, 3D interpolation

```
title Atlas stellar atmosphere, 3D interpolation
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the atlas 3dim model option.
# I choose the T_eff and log(g) values arbitrarily.
table star atlas 3-dim 38400.0 4.82 -1.42
luminosity 4.509202522 solar
table star atlas odfnew 3-dim 38400.0 4.82 0.42
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas_3d.per"
save overview last "stars_atlas_3d.ovr"
save results last "stars_atlas_3d.rlt"
save transmitted continuum last "stars_atlas_3d.trn" no header
save continuum last "stars_atlas_3d.con" units angstrom
#
# stars_atlas_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Atlas model atmosphere continua.

Checks: table star atlas 3dim command works.

`stars_atlas_all.in`

interpolate on Atlas grids

```
title interpolate on Atlas grids
#
# commands controlling continuum =========
# Include stars with a wide range of metallicities to test access to these grids.
table star atlas Z+1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.3 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.1 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.1 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.3 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-1.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-2.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-2.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-3.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-3.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-4.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-4.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-5.0 38400.0 4.82
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
```

```
# commands controlling output =========
#
save performance "stars_atlas_all.per"
save overview last "stars_atlas_all.ovr"
save results last "stars_atlas_all.rlt"
save transmitted continuum last "stars_atlas_all.trn" no header
save continuum last "stars_atlas_all.con" units angstrom
#
# stars_atlas_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the 2D grids of various metallicity of Atlas model atmosphere continua.

Checks: access to the various atlas grids

`stars_atlas_odfnew_all.in`

access various Atlas ODFNEW grids

```
title access various Atlas ODFNEW grids
#
# commands controlling continuum =========
# Include stars with a wide range of metallicities to test access to these grids.
table star atlas odfnew Z+0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z+0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z+0.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-1.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-2.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-2.5 38400.0 4.82
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas_odfnew_all.per"
save overview last "stars_atlas_odfnew_all.ovr"
save results last "stars_atlas_odfnew_all.rlt"
save transmitted continuum last "stars_atlas_odfnew_all.trn" no header
save continuum last "stars_atlas_odfnew_all.con" units angstrom
#
```

```
# stars_atlas_odfnew_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the Atlas ODFNEW model atmosphere continua.

Checks: access to the various atlas odfnew grids

---

stars_bstar2006.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily.
table star tlusty bstar 20400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_bstar2006.per"
save overview last "stars_bstar2006.ovr"
save results last "stars_bstar2006.rlt"
save continuum last "stars_bstar2006.con" units angstrom
save transmitted continuum last "stars_bstar2006.trn" no header
#
# stars_bstar2006.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar command works.

---

stars_bstar2006_3d.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty bstar 3-dim 20400.0 4.2 -0.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_bstar2006_3d.per"
save overview last "stars_bstar2006_3d.ovr"
save results last "stars_bstar2006_3d.rlt"
save continuum last "stars_bstar2006_3d.con" units angstrom
save transmitted continuum last "stars_bstar2006_3d.trn" no header
#
# stars_bstar2006_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar 3-dim command works.

---

stars_bstar2006_all.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of 6 B stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the BSTAR 2006 grids. I choose the T_eff
# and log(g) values arbitrarily.
table star tlusty bstar Z+0.3 20000.0 4.5
luminosity 4.509202522 solar
table star tlusty bstar Z+0.0 21400.0 4.5
luminosity 4.509202522 solar
table star tlusty bstar Z-0.3 15000.0 4.2
luminosity 4.509202522 solar
table star tlusty bstar Z-0.7 20400.0 4.2
luminosity 4.509202522 solar
```

```
table star tlusty bstar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty bstar Z-INF 18000.0 4.75
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_bstar2006_all.per"
save overview last "stars_bstar2006_all.ovr"
save results last "stars_bstar2006_all.rlt"
save continuum last "stars_bstar2006_all.trn" units angstrom
save transmitted continuum last "stars_bstar2006_all.trn" no header
#
# stars_bstar2006_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar metallicity option works.

`stars_costar1.in`

costar interpolation mode 1

```
title costar interpolation mode 1
#
# commands controlling continuum =========
table star costar, 40000 K
ionization parameter -2
table star costar, 31000 K, index 4
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 6000K
no blends
```

```
#
# commands controlling output =========
save overview "stars_costar1.ovr"
save performance "stars_costar1.per"
save continuum last "stars_costar1.con" units angstrom
#
# stars_costar1.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

`stars_costar2.in`

costar interpolation mode 2

```
title costar interpolation mode 2
#
# commands controlling continuum =========
table star costar 35575.4 4.2367
ionization parameter -2
table star costar 34468.5 3.86765
ionization parameter -2
table star costar 41741.2 4.02
ionization parameter -2
table star costar 45000 4.1593
ionization parameter -2
table star costar 27500 3.3
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar2.ovr"
save performance "stars_costar2.per"
save continuum last "stars_costar2.con" units angstrom
#
# stars_costar2.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

`stars_costar3.in`

costar interpolation mode 3

```
title costar interpolation mode 3
#
# commands controlling continuum =========
table star costar zams 40.0 Msol 2.85e6
ionization parameter -2
table star costar zams 40.0 Msol 4e6
ionization parameter -2
table star costar zams 50.9 Msol 2.85e6
ionization parameter -2
table star costar zams 42.9 Msol 1.6e6
ionization parameter -2
table star costar zams 70.5 Msol 2.1e6
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar3.ovr"
save performance "stars_costar3.per"
save continuum last "stars_costar3.con" units angstrom
#
# stars_costar3.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

---

stars_costar4.in

costar interpolation mode 4

```
title costar interpolation mode 4
#
# commands controlling continuum =========
table star costar age 2.85e6 40.0
ionization parameter -2
table star costar age 4e6 40.0
ionization parameter -2
table star costar age 2.85e6 50.9
ionization parameter -2
table star costar age 1.6e6 42.9
ionization parameter -2
table star costar age 2.1e6 70.5
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
```

```
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar4.ovr"
save performance "stars_costar4.per"
save continuum last "stars_costar4.con" units angstrom
#
# stars_costar4.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

---

stars_costarhalo.in

costar halo abundances

```
title costar halo abundances
#
# commands controlling continuum =========
table star costar, halo abundances, 40000 K
ionization parameter -2
#
# commands for density & abundances =========
hden 2
abundances ism
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 6900K
no blends
#
# commands controlling output =========
save overview "stars_costarhalo.ovr"
save performance "stars_costarhalo.per"
save continuum last "stars_costarhalo.con" units angstrom
#
#
# stars_costarhalo.in
# class stars
# ======================================
#
```

This test checks that the code can read the CoStar stellar atmospheres. It checks the resulting ionization to make sure that the continuum shape is ok. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

---

stars_kurucz79.in

Kurucz 1979 SED

```
title Kurucz 1979 SED
```

```
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star kurucz 30400.0
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_kurucz79.per"
save overview last "stars_kurucz79.ovr"
save results last "stars_kurucz79.rlt"
save transmitted continuum last "stars_kurucz79.trn" no header
save continuum last "stars_kurucz79.con" units angstrom
#
# stars_kurucz79.in
# class stars
# ======================================
```

This is a test that the code can correctly access the Kurucz model atmosphere continua described by Kurucz (1979). Kevin Volk provided it as part of his original coding of these stellar atmosphere files. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

Checks: table star kurucz command works.

`stars_mihalas.in`

Mihalas SED

```
title Mihalas SED
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star mihalas 30400.0
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
```

```
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_mihalas.per"
save overview last "stars_mihalas.ovr"
save results last "stars_mihalas.rlt"
save transmitted continuum last "stars_mihalas.trn" no header
save continuum last "stars_mihalas.con" units angstrom
#
# stars_mihalas.in
# class stars
# ======================================
```

This is a test that the code can correctly access the small Mihalas grid of NLTE model atmospeheres Constant temperature is assumed since this tests shape of continuum not thermal physics.

Checks: table star mihalas command works.

`stars_obstar_merged.in`

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily.
table star tlusty obstar 20400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_obstar_merged.per"
save overview last "stars_obstar_merged.ovr"
save results last "stars_obstar_merged.rlt"
save continuum last "stars_obstar_merged.con" units angstrom
save transmitted continuum last "stars_obstar_merged.trn" no header
#
```

```
# stars_obstar_merged.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar command works.

`stars_obstar_merged_3d.in`

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty obstar 3-dim 20400.0 4.2 -0.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_obstar_merged_3d.per"
save overview last "stars_obstar_merged_3d.ovr"
save results last "stars_obstar_merged_3d.rlt"
save continuum last "stars_obstar_merged_3d.con" units angstrom
save transmitted continuum last "stars_obstar_merged_3d.trn" no header
#
# stars_obstar_merged_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar 3-dim command works.

`stars_obstar_merged_all.in`

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of 6 B stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the BSTAR 2006 grids. I choose the T_eff
# and log(g) values arbitrarily.
table star tlusty obstar Z+0.3 40000.0 4.5
luminosity 4.509202522 solar
table star tlusty obstar Z+0.0 21400.0 4.5
luminosity 4.509202522 solar
table star tlusty obstar Z-0.3 35000.0 4.2
luminosity 4.509202522 solar
table star tlusty obstar Z-0.7 20400.0 4.2
luminosity 4.509202522 solar
table star tlusty obstar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty obstar Z-INF 18000.0 4.75
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_obstar_merged_all.per"
save overview last "stars_obstar_merged_all.ovr"
save results last "stars_obstar_merged_all.rlt"
save continuum last "stars_obstar_merged_all.trn" units angstrom
save transmitted continuum last "stars_obstar_merged_all.trn" no header
#
# stars_obstar_merged_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar metallicity option works.

`stars_optimize1.in`

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star tlusty ostar 3-dim 31200 3.6 -1.12 vary
```

```
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
optimize iteration 750
# the following spectrum was derived by running this sim at hden 5, t=4,
# and T_star=51200
# resulting eden was 5.040 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0446
O 2 3726.03 0.1164
Blnd 7323 0.1237
Blnd 7332 0.1018
O 3 5006.84 10.0205
O 3 4363.21 0.0968
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "stars_optimize1.ovr"
save performance "stars_optimize1.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for Teff. The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, T_star = 51200 K.

`stars_optimize2.in`

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star costar 36200 vary
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
```

```
optimize iteration 500
# the following spectrum was derived by running this sim at hden 5, t=4,
# and T_star=51200
# resulting eden was 5.041 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0365
O 2 3726.03 0.0951
Blnd 7323 0.1012
Blnd 7332 0.0833
O 3 5006.84 10.4461
O 3 4363.21 0.1010
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "stars_optimize2.ovr"
save performance "stars_optimize2.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for Teff. The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, T_star = 51200 K.

`stars_optimize3.in`

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star costar age 5.8 log 36 msol vary
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
optimize iteration 500
# the following spectrum was derived by running this sim at hden 5, t=4,
# and log(age)=6.3
# resulting eden was 5.040 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0680
O 2 3726.03 0.1774
Blnd 7323 0.1887
Blnd 7332 0.1554
O 3 5006.84 8.7015
O 3 4363.21 0.0841
end of lines
#
# commands controlling output =========
print line faint -2
```

```
#
save overview "stars_optimize3.ovr"
save performance "stars_optimize3.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for log(age). The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, log(age/yr) = 6.3.

---

stars_ostar2002.in

tlusty O star grid

```
title tlusty O star grid
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star tlusty ostar 30400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_ostar2002.per"
save overview last "stars_ostar2002.ovr"
save results last "stars_ostar2002.rlt"
save continuum last "stars_ostar2002.con" units angstrom
save transmitted continuum last "stars_ostar2002.trn" no header
#
# stars_ostar2002.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar command works.

---

stars_ostar2002_3d.in

tlusty Ostar grid

```
title tlusty Ostar grid
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty ostar 3-dim 30400.0 4.2 -1.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_ostar2002_3d.per"
save overview last "stars_ostar2002_3d.ovr"
save results last "stars_ostar2002_3d.rlt"
save continuum last "stars_ostar2002_3d.con" units angstrom
save transmitted continuum last "stars_ostar2002_3d.trn" no header
#
# stars_ostar2002_3d.in
# class stars
# ========================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar 3-dim command works.

`stars_ostar2002_all.in`

tlusty Ostar grid

```
title tlusty Ostar grid
#
# commands controlling continuum =========
# Approximate model of 10 hot stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the OSTAR 2002 grids. I choose the T_eff
# and log(g) values such that the selection algorithm gets a good workout.
table star tlusty ostar Z+0.3 30000.0 4.5
luminosity 4.509202522 solar
table star tlusty ostar Z+0.0 31400.0 4.5
luminosity 4.509202522 solar
```

```
table star tlusty ostar Z-0.3 45000.0 4.2
luminosity 4.509202522 solar
table star tlusty ostar Z-0.7 30400.0 4.2
luminosity 4.509202522 solar
table star tlusty ostar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty ostar Z-1.5 55000.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z-1.7 27500.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z-2.0 55000.0 3.00
luminosity 4.509202522 solar
table star tlusty ostar Z-3.0 44400.0 3.2
luminosity 4.509202522 solar
table star tlusty ostar Z-INF 53000.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z+0.0 48400.0 3.87
luminosity 4.509202522 solar
table star tlusty ostar Z-0.7 48400.0 3.55
luminosity 4.509202522 solar
table star tlusty ostar Z+0.3 43400.0 3.65
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_ostar2002_all.per"
save overview last "stars_ostar2002_all.ovr"
save results last "stars_ostar2002_all.rlt"
save continuum last "stars_ostar2002_all.con" units angstrom
save transmitted continuum last "stars_ostar2002_all.trn" no header
#
# stars_ostar2002_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar metallicity option works, also test selection algorithm.

`stars_rauch_3d.in`

Rauch 3-dimensional grid

```
title Rauch 3-dimensional grid
#
```

```
# commands controlling continuum =========
table star rauch 3-dim T = 150000 K, g = 6.5 , log(Z) = -0.6
luminosity 4.5 solar
table star rauch old 3-dim T = 233000 K, g = 7.5 , log(Z) = -0.32
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_3d.per"
save overview last "stars_rauch_3d.ovr"
save results last "stars_rauch_3d.rlt"
save continuum last "stars_rauch_3d.con" units angstrom
#
# stars_rauch_3d.in
# class stars
# ======================================
```

This model checks that the code is able to access the 3-dim versions of the Rauch grids of stellar atmosphere models. Constant temperature is set since this test is intended to test shape of ionizing continuum, not thermal physics.

`stars_rauch_cowd.in`

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch co wd T = 238000 K
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
# test adding continuum points
set nfnu add 10 cm
set nfnu add 350 micron
set nfnu add 200 angstrom
#
# commands controlling output =========
save performance "stars_rauch_cowd.per"
save overview last "stars_rauch_cowd.ovr"
save results last "stars_rauch_cowd.rlt"
```

```
save continuum last "stars_rauch_cowd.con" units angstrom
#
# stars_rauch_cowd.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the C/O white dwarf version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_h+he.in

Rauch PN central star

```
title Rauch PN central star
#
# commands controlling continuum =========
# this tests the various interpolation modes of the 3d grid
table star rauch h+he T = 150000 K, g = 6.5 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.5 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.25 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.5 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.25 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.5 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.25 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.25 , f(He) = 0.25
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_h+he.per"
save overview last "stars_rauch_h+he.ovr"
save results last "stars_rauch_h+he.rlt"
save continuum last "stars_rauch_h+he.con" units angstrom
#
# stars_rauch_h+he.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H+He version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_h-ca.in

Rauch central star hot PN

```
title Rauch central star hot PN
# NB
# this uses the H-Ca rauch atmospheres
#
# commands controlling continuum =========
table star old rauch T = 250000 K, g = 7.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# other commands for details =========
no level2
no blends
#
# commands for density & abundances =========
hden 3.0
abundances planetary
#
# commands controlling output =========
save performance "stars_rauch_h-ca.per"
save overview last "stars_rauch_h-ca.ovr"
save results last "stars_rauch_h-ca.rlt"
save continuum last "stars_rauch_h-ca.con" units angstrom
#
# stars_rauch_h-ca.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H-Ca Rauch grid of stellar atmosphere models.

`stars_rauch_h-ni.in`

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch T = 150000 K, g = 6.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_h-ni.per"
```

```
save overview last "stars_rauch_h-ni.ovr"
save results last "stars_rauch_h-ni.rlt"
save continuum last "stars_rauch_h-ni.con" units angstrom
#
# stars_rauch_h-ni.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H-Ni version of the Rauch grid of stellar atmosphere models. Constant temperature is set since this test is intended to test shape of ionizing continuum, not thermal physics.

`stars_rauch_helium.in`

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch helium T = 240000 K, g = 8.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
# test adding continuum points
set nfnu add 10 cm
set nfnu add 350 micron
set nfnu add 200 angstrom
#
# commands controlling output =========
save performance "stars_rauch_helium.per"
save overview last "stars_rauch_helium.ovr"
save results last "stars_rauch_helium.rlt"
save continuum last "stars_rauch_helium.con" units angstrom
#
# stars_rauch_helium.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the pure helium version of the Rauch grid of stellar atmosphere models.

`stars_rauch_hydr.in`

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
```

```
table star rauch hydr T = 240000 K, g = 8.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_hydr.per"
save overview last "stars_rauch_hydr.ovr"
save results last "stars_rauch_hydr.rlt"
save continuum last "stars_rauch_hydr.con" units angstrom
#
# stars_rauch_hydr.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the pure hydrogen version of the Rauch grid of stellar atmosphere models.

`stars_rauch_pg1159.in`

Rauch hot [WR] PN

```
title Rauch hot [WR] PN
#
# commands controlling continuum =========
table star rauch pg1159 T=150000K g=6.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_pg1159.per"
save overview last "stars_rauch_pg1159.ovr"
save results last "stars_rauch_pg1159.rlt"
save continuum last "stars_rauch_pg1159.con" units angstrom
#
# stars_rauch.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the PG1159 version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_pg1159_ascii.in

Rauch cool [WR] PN

```
title Rauch cool [WR] PN
#
# commands controlling continuum =========
table star "rauch_pg1159.ascii" T=40000K g=7
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
set nfnu add 9.5 angstrom
no blends
#
# commands controlling output =========
save performance "stars_rauch_pg1159_ascii.per"
save overview last "stars_rauch_pg1159_ascii.ovr"
save results last "stars_rauch_pg1159_ascii.rlt"
save continuum last "stars_rauch_pg1159_ascii.con" units angstrom
#
# stars_rauch_pg1159_ascii.in
# class stars
# ========================================
```

This is a model of a cool PNCS, and checks that the code can correctly rebin a model with zero fluxes embedded. It also exercises reading directly from an ascii file.

---

stars_starburst99.in

Starburst 99 SED

```
title Starburst 99 SED
#
# commands controlling continuum =========
# read the table starburst and interploate to an age of 1e8 years
table star log age=8 "starburst99.mod"
luminosity 43
# add background continuum - starburs 99 does not extend
# into fir so code would complain about zero continuum
# adding the cosmic background stops this complaint
background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
stop zone 1
```

```
radius 20
#
# other commands for details =========
constant temper 4
no blends
#
# commands controlling output =========
save overview "stars_starburst99.ovr"
save performance "stars_starburst99.per"
save continuum last "stars_starburst99.con" units angstrom
#
#
# stars_starburst99.in
# class stars
# ======================================
#
```

this is a demonstration of the use of a Starburst 99 spectrum. It was provided to me by anand Srianand, and we used it in Srianand et al. 2003. A constant temperature is set since this is to test shape of continuum not thermal physics. It also tests access to user-supplied grids as the mechanism is the same.

`stars_starburst99_2d.in`

Starburst 99 2D SED

```
title Starburst 99 2D SED
#
# commands controlling continuum =========
# read the table starburst and interpolate to an age of 2.09e6 years
# and a metallicity of 12.
table star log age=6.32 Z=12. "starburst99_2d.mod"
luminosity 43
# add background continuum - starburs 99 does not extend
# into fir so code would complain about zero continuum
# adding the cosmic background stops this complaint
background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
stop zone 1
radius 20
#
# other commands for details =========
constant temper 4
no blends
#
# commands controlling output =========
save overview "stars_starburst99_2d.ovr"
save performance "stars_starburst99_2d.per"
save continuum last "stars_starburst99_2d.con" units angstrom
#
#
# stars_starburst99_2d.in
# class stars
# ======================================
#
```

this is a demonstration of the use of a manually crafted Starburst 99 2D grid, allowing for interpolation in both age and metallicity. It was provided by Christophe Morisset. A constant temperature is set since this is to test shape of continuum not thermal physics. It also tests access to user-supplied grids as the mechanism is the same.

---

stars_werner.in

Werner stars grid

```
title Werner stars grid
#
# commands controlling continuum =========
table star werner 190000 g=7.5
luminosity total 38
#
# commands for density & abundances =========
hden 4
abundances planetary no grains
grains agm no qheat single
#
# commands controlling geometry =========
radius 17
sphere
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 4.373
no blends
#
# commands controlling output =========
#
save performance "stars_werner.per"
save overview last "stars_werner.ovr"
save results last "stars_werner.rlt"
save continuum last "stars_werner.con" units angstrom
save transmitted continuum last "stars_werner.trn"
#
# stars_werner.in
# class stars
# ========================================
#
```

This checks that the code can access Kevin Volk39s Werner atmospheres.

Checks:
- table star Werner atmosphere works. constant temperature is set to that this tests shape of stellar continuum

---

stars_wmbasic.in

wmbasic stellar SED

```
title wmbasic stellar SED
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the WMBASIC model option.
# I choose the T_eff, log(g), and log(Z) values arbitrarily.
table star wmbasic 30000.0 4.0 -0.3
luminosity 4.509202522 solar
table star wmbasic 32000.0 4.0 0.0
luminosity 4.509202522 solar
table star wmbasic 40000.0 3.6 -0.3
luminosity 4.509202522 solar
table star wmbasic 35000.0 4.0 -0.15
luminosity 4.509202522 solar
```

```
table star wmbasic 57000.0 4.0 0.0
luminosity 4.509202522 solar
table star wmbasic 37000.0 3.4 -0.3
luminosity 4.509202522 solar
table star wmbasic 32000.0 4.0 -0.1
luminosity 4.509202522 solar
table star wmbasic 36000.0 3.5 -0.12
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly
# by the stellar continuum; disable this process to avoid critical
# dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_wmbasic.per"
save overview last "stars_wmbasic.ovr"
save results last "stars_wmbasic.rlt"
save transmitted continuum last "stars_wmbasic.trn" no header
save continuum last "stars_wmbasic.con" units angstrom
save continuum bins last "stars_wmbasic.bin" no header
#
# stars_wmbasic.in
# class stars
# ======================================
```

This is a test that the code can correctly access the WMBASIC O-star model atmosphere continua.

Checks: table star wmbasic command works.

---

thin.in

"Thin coronal model"

```
title "Thin coronal model"
coronal equilibrium 1e6K
hden 0
stop thickness 0
iterate
save performance "thin.per"
# thin.in
# ==========================
```

This tests whether a layer with thickness much smaller than any relevant lengthscale is modelled in a single zone

---

time_cool_cd.in

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e4 K
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cd"
save time dependent ".tim" no hash
save dt ".dt" no hash
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
# time_cool_cd.in
# class dynamics
# ======================================
#
```

test time dependent cooling at constant density

`time_cool_cd_eq.in`

constant density equilibrium cooling cloud

```
title constant density equilibrium cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
```

```
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e4 K
# this will do equilibrium cooling
set dynamics populations equilibrium
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cd_eq"
save time dependent ".tim" no hash
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
# time_cool_cd_eq.in
# class dynamics
# ========================================
#
```

test time dependent equilibrium cooling at constant density

`time_cool_cd_flux.in`

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e7 K
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set cumulative flux
set save prefix "time_cool_cd_flux"
#
# commands giving the asserts =========
#
# time_cool_cd_flux.in
# class dynamics
```

```
# ======================================
#
```

Test time dependent cooling at constant density. In time_cool_cd.in, the line emission accumulation is done by default by mass. In this sim, the accumulation is done by flux (see 'set cumulative' above). This sim is meant simply to exercise the 'set cumulative flux' command, so a full run to low temperatures is deemed unnecessary.

`time_cool_cd_noaccu.in`

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e7 K
cosmic rays background
#
# commands controlling output =========
normalize to "O 8" 18.9689A
print line faint -3 log
print ages
set cumulative off
set save prefix "time_cool_cd_noaccu"
#
# commands giving the asserts =========
#
# time_cool_cd_flux.in
# class dynamics
# ======================================
#
```

Test time dependent cooling at constant density. In time_cool_cd.in, the line emission accumulation is done by default by mass. In this sim, no accumulation is performed (see 'set cumulative' above). The final line fluxes are those of the last iteration. This sim is meant simply to exercise the 'set cumulative off' command, so a full run to low temperatures is deemed unnecessary.

D.4 The Slow Test Suite

Table D.3 lists the simulations in the `slow` test directory.

Table D.3: The simulations in the slow test suite.

Class	Function
dynamics_HII_PDR	fast H+He+metals (low ionization parameter) 009 km s
feii_blr_n09_p18	FeII model
feii_blr_n09_p18_Z20	FeII model
feii_blr_n11_p20	FeII model
feii_blr_n11_p20_Z20	FeII model
feii_blr_n12_p19	FeII model
feii_blr_n12_p19_Z20	FeII model
feii_blr_n12_p21	FeII model
feii_blr_n12_p21_Z20	FeII model
feii_blr_n13_p18	BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
feii_blr_n13_p18_Z20	BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
feii_blr_n13_p22	FeII model
feii_blr_n13_p22_Z20	FeII model
grid_extreme	exercise full range of density, temperature
h2_HTT91	Hollenbach et al. 1991 low-density PDR
h2_orion_bar	Title Orion Bar with magneitc field with equipartition cosmic rays
h2_orion_hii_pdr	constant gas pressure orion into pdr
h2_pdr_leiden_f2	low density high flux model 2 as defined in e-mail
h2_pdr_leiden_f3	high density low flux model 3 as defined in e-mail
h2_pdr_leiden_f4	high density high flux model 4 as defined in e-mail
h2_pdr_leiden_hack_f1	low density low flux model 1 as defined in e-mail
h2_pdr_leiden_v1	model 5 as defined in e-mail
h2_pdr_leiden_v2	model 6 as defined in e-mail
h2_pdr_leiden_v3	model 7 as defined in e-mail
h2_pdr_leiden_v4	model 8 as defined in e-mail
h2_th85orion	Tielens and Hollenbach pdr model with orion grains, Table 2, paper b
m17_p07	Pellegrini+07 2007ApJ...658.1119P model for M17
orion_hii_pdr_pp	the Orion HII Region / PDR / Molecular cloud with an open geometry
pdr_xdr	XDR sim
time_cool_cp	constant pressure cooling cloud
time_cool_cp_eq	constant pressure equilibrium cooling cloud

This HTML file was created by the program doc_tsuite.pl, doc_tsuite.txt contains a tab delimited list of the files.

---

dynamics_HII_PDR.in

fast H+He+metals (low ionization parameter) 009 km s

```
title fast H+He+metals (low ionization parameter) 009 km s
failures 1
wind -9 advection no continuum
set dynamics pressure mode subsonic
iterate 10 to convergence 0.001
set nend 2000
blackbody 120000
phi(h) 9.5
sphere
turbulence 8 km/sec
normalize to "Q(H)" 4861.32A
hden 3.5
init "ism.ini"
abundances hii region no grains
grains orion no qheat single
stop thickness 18
stop efrac -3
stop temperature off
stop Av point 0.0333
no molecules
database h-like levels small
database he-like levels small
print lines emergent off
save performance "dynamics_HII_PDR.per"
save dr "dynamics_HII_PDR.dr"
save overview "dynamics_HII_PDR.ovr"
save wind "dynamics_HII_PDR.wnd"
#
# dynamics_HII_PDR.in
#
```

---

feii_blr_n09_p18.in

FeII model

```
title FeII model
table agn
species "Fe+" levels=all
print lines column
print lines sort intensity
hden 9
phi(h) 18
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n09_p18"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column densities ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
```

```
save dr ".dr" last
save convergence reason ".cvr"
# This is one of the 5 models that sample the LOC plane.
```

---

feii_blr_n09_p18_Z20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
abundances starburst 20
hden 9
phi(h) 18
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n09_p18_Z20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n11_p20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
hden 11
phi(h) 20
stop column density 23
iterate to convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n11_p20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n11_p20_Z20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
failures 2
abundances starburst 20
hden 11
phi(h) 20
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n11_p20_Z20"
save performance ".per"
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species lines ".lin" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save heating ".het"
save cooling ".col"
save element calcium ".ca"
save overview ".ovr" last
save convergence reason ".cvr"
save dr ".dr" last
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n12_p19.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
hden 12
phi(h) 19
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n12_p19"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n12_p19_Z20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
abundances starburst 20
hden 12
phi(h) 19
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n12_p19_Z20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n12_p21.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
hden 12
phi(h) 21
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n12_p21"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the models that sample the LOC plane.

---

feii_blr_n12_p21_Z20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
abundances starburst 20
species "Fe+" levels=all
hden 12
phi(h) 21
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n12_p21_Z20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the models that sample the LOC plane.

`feii_blr_n13_p18.in`

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
print lines column
print lines sort intensity
species "Fe+" levels=all
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
table agn
hden 13
phi(h) 18
stop column density 22
double
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n13_p18"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n13_p18_Z20.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
print lines column
print lines sort intensity
species "Fe+" levels=all
abundances starburst 20
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
table agn
hden 13
phi(h) 18
stop column density 19
double
iterate convergence limit 15
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n13_p18_Z20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n13_p22.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
hden 13
phi(h) 22
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n13_p22"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
save heating ".het" last
save cooling ".coo" last
```

This is one of the 5 models that sample the LOC plane.

---

feii_blr_n13_p22_Z20.in

FeII model

```
title FeII model
table agn
print lines column
print lines sort intensity
species "Fe+" levels=all
abundances starburst 20
hden 13
phi(h) 22
stop column density 23
iterate convergence
normalize to "H 1" 1215.67A 100
init "c84.ini"
set save prefix "feii_blr_n13_p22_Z20"
save performance ".per"
save species lines ".lin" "Fe+" last
save species continuum units microns ".fe2con" "Fe+" last
save species column density ".fe2col" "Fe+[:]" last
save species densities ".lev" "Fe+[:]" last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
save overview ".ovr" last
save dr ".dr" last
save convergence reason ".cvr"
save heating ".het"
save cooling ".col"
```

This is one of the 5 models that sample the LOC plane.

---

grid_extreme.in

exercise full range of density, temperature

```
title exercise full range of density, temperature
set save prefix "grid_extreme"
#
element lithium off
element berylium off
element boron off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 6 vary
# do not run in parallel so we have good performance statistics
grid 1 6 1 sequential
# -8 18
hden 2 vary
grid -8 18 1
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
```

```
print lines emergent off
save performance no hash ".per"
save grid no hash ".grd" last
save overview last no hash ".ovr" last
save average ".avr" last
temperature hydrogen 2
end of average
#
#
# grid_extreme.in limits
# Figs 17&18 of 2013RMxAA..49..137F
```

---

h2_HTT91.in

Hollenbach et al. 1991 low-density PDR

```
title Hollenbach et al. 1991 low-density PDR
iterate
#
#
hden 3
#
# this is hot star continuum
black 30000
intensity 0.2 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
turbulence 1.5 km/sec
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
grains orion, abundance log 0.16
grains PAH
database h2
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
normalize to "C 2" 157.636m
sphere
Database H-like Lyman pumping off
cosmic rays, background
# stop when gas is fully neutral
stop efrac -10
# this is to stop at an intended place, since results would be
# very dependent on details if we stop on temperature
stop thickness 18.954
# stop when gas is cold
stop temperature 10 linear
# add this to mimic unmodelled neutral gas
double optical depths
#
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
#
save performance "h2_HTT91.per"
save overview last "h2_HTT91.ovr"
save dr "h2_HTT91.dr"
save molecules last "h2_HTT91.mol"
save results last "h2_HTT91.rlt"
save continuum units microns last "h2_HTT91.con"
save heating last "h2_HTT91.het"
save cooling last "h2_HTT91.col"
save chemistry rates destruction "h2_HTT91.H2d" "H2"
save chemistry rates creation "h2_HTT91.H2c" "H2"
```

```
#
# h2_HTT91.in
```

This is the Hollenbach et al 1991 Low-density PDR The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

there is very little CO in this model since it is not thick enough for the UV pumping lines to become optically thick

---

h2_orion_bar.in

Title Orion Bar with magneitc field with equipartition cosmic rays

```
Title Orion Bar with magneitc field with equipartition cosmic rays
# This is the Orion Bar model presented in Pellegrini et al, Shaw et al.
#
# commands controlling continuum =========
# these give the shape and intensity
table SED "star_kurucz_39600.dat"
Q(H) 48.99
brems 6
luminosity 32.6 range 36.76 to 588.0 Ryd
#
# commands for density & abundances =========
Hden 3.500
init file="ism.ini"
Abundances H II region no grains
grains orion no qheat
# these were actually used in the paper
grains PAH no qheat
#
# commands controlling geometry =========
iterate
sphere
double
stop temperature 0.602K
Constant pressure
Magnetic field tangled -5.10 2
radius 0.114 to 0.5 linear parsecs
#
# other commands for details =========
cosmic rays equipartition
Set nend 3000
database h2
# use ORNL data for ortho & para H2 collisions
database H2 orH2 collisions ORNL
database H2 paH2 COLLISIONS ORNL
turbulence 2km/s 2
#
# commands controlling output =========
print line faint -6
print line sort wavelength
print line column
print last
save performance "h2_orion_bar.per"
save grain opacity "h2_orion_bar.grop"
save h2 populations zone last "h2_orion_bar.h2pop"
save continuum last "h2_orion_bar.con" units microns
save H2 lines last "h2_orion_bar.h2lin"
save overview last "h2_orion_bar.ovr"
save pressure last "h2_orion_bar.press"
save molecules last "h2_orion_bar.mol"
save secondaries last "h2_orion_bar.2nd"
save heating last "h2_orion_bar.heat"
save H2 rates last "h2_orion_bar.h2rat" last
```

```
save h2 column density last "h2_orion_bar.h2col"
save h2 temperature last "h2_orion_bar.temp"
save PDR last "h2_orion_bar.pdr"
#
#
# hii pdr h2_orion_bar.in
# ======================================
#
```

This is the Orion Bar model discussed by Pellegrini, E. W.; Baldwin, J. A.; Ferland, G. J.; Shaw, G.; Heathcote, S. ApJ, 693, 285 2009ApJ...693..285P and Shaw, Gargi; Ferland, G. J.; Henney, W. J.; Stancil, P. C.; Abel, N. P.; Pellegrini, E. W.; Baldwin, J. A.; van Hoof, P. A. M. 2009arXiv0906.2310S

`h2_orion_hii_pdr.in`

constant gas pressure orion into pdr

```
title constant gas pressure orion into pdr
stop temperature 10 linear
#
# print lots of faint CO lines
print line faint -6
print lines column
print lines sort wavelength
stop AV 1000 point
constant gas pressure
sphere
#
# the incident continuum is two parts
# star and flux of photons striking it
table SED "star_kurucz_39600.dat"
#
Q(H) 49
radius 17.4507
# plus hot brems
brems 6
phi(h) 10
#
# add cosmic rays, which are important at depth
cosmic rays, background
#
# we have a spherical geometry but want to simulate observing
# through a spectrometer's slit. use the aperture
# command for this
aperture beam
#
# the observed microturbulence
turbulence 8 km/sec no pressure
#
# density and abundances
hden 4
init file="ism.ini"
abundances hii region no grains
grains orion
grains pah
database h2
#
set nend 2000
#
save performance "h2_orion_hii_pdr.per"
save overview last "h2_orion_hii_pdr.ovr"
save hydrogen 21 cm last "h2_orion_hii_pdr.21cm"
save heating "h2_orion_hii_pdr.het"
save cooling "h2_orion_hii_pdr.col"
save dr last "h2_orion_hii_pdr.dr"
```

```
save results last "h2_orion_hii_pdr.rlt"
save continuum last "h2_orion_hii_pdr.con" units microns
save hydrogen lya last "h2_orion_hii_pdr.lya"
save grain charge last "h2_orion_hii_pdr.grnchr"
save grain potential last "h2_orion_hii_pdr.grnpot"
save H2 lines last "h2_orion_hii_pdr.h2lin"
save H2 column density last "h2_orion_hii_pdr.h2col"
save chemistry rates destruction "h2_orion_hii_pdr.H2d" "H2"
save chemistry rates creation "h2_orion_hii_pdr.H2c" "H2"
save molecules "h2_orion_hii_pdr.mol"
#
# h2_orion_hii_pdr.in
```

05 dec 19, had stopped at 1 pc, gas/dust got very cold and H2 stopped forming, H2 went to H0 - this below the CO network out of the water. stop at AV of 1000 instead. Is this loss of H2 at low grain temperature physical? Is it ever seen?

---

h2_pdr_leiden_f2.in

low density high flux model 2 as defined in e-mail

```
title low density high flux model 2 as defined in e-mail
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use
# half the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
database h2
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "h2_pdr_leiden_f2.per"
save overview "h2_pdr_leiden_f2.ovr"
save leiden lines "h2_pdr_leiden_f2.lin"
save leiden "h2_pdr_leiden_f2.lei"
save dr "h2_pdr_leiden_f2.dr"
save grain physical conditions "h2_pdr_leiden_f2.grn"
save H2 lines "h2_pdr_leiden_f2.h2lin" all
save H2 column density "h2_pdr_leiden_f2.h2col"
save H2 populations matrix zone "h2_pdr_leiden_f2.pop"
save chemistry rates destruction "h2_pdr_leiden_f2.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_f2.H2c" "H2"
#
#
# h2_pdr_leiden_f2.in
# class pdr
# ======================================
#
```

h2_pdr_leiden_f3.in

high density low flux model 3 as defined in e-mail

```
title high density low flux model 3 as defined in e-mail
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# ice formation is exteme and will establish the thickness, which would
# make this very sensitive to details - turn off ices
no grain molecules
database h2
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "h2_pdr_leiden_f3.per"
save overview "h2_pdr_leiden_f3.ovr"
save leiden lines "h2_pdr_leiden_f3.lin"
save leiden "h2_pdr_leiden_f3.lei"
save dr "h2_pdr_leiden_f3.dr"
save grain physical conditions "h2_pdr_leiden_f3.grn"
save H2 lines "h2_pdr_leiden_f3.h2lin" all
save H2 column density "h2_pdr_leiden_f3.h2col"
save H2 populations matrix zone "h2_pdr_leiden_f3.pop"
save H2 rates "h2_pdr_leiden_f3.rat"
save chemistry rates destruction "h2_pdr_leiden_f3.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_f3.H2c" "H2"
#
#
# h2_pdr_leiden_f3.in
# class pdr
# ========================================
#
```

---

h2_pdr_leiden_f4.in

high density high flux model 4 as defined in e-mail

```
title high density high flux model 4 as defined in e-mail
#
# commands controlling continuum =========
#
```

```
# commands for density & abundances =========
grains ism 1.16 no qheat
#
# commands controlling geometry =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# hydrogen density
hden 5.5
#
# other commands for details =========
database h2
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "h2_pdr_leiden_f4.per"
save overview "h2_pdr_leiden_f4.ovr"
save leiden lines "h2_pdr_leiden_f4.lin"
save leiden "h2_pdr_leiden_f4.lei"
save dr "h2_pdr_leiden_f4.dr"
save grain physical conditions "h2_pdr_leiden_f4.grn"
save H2 lines "h2_pdr_leiden_f4.h2lin" all
save H2 column density "h2_pdr_leiden_f4.h2col"
save H2 populations matrix zone "h2_pdr_leiden_f4.pop"
save H2 solomon "h2_pdr_leiden_f4.sol"
save chemistry rates destruction "h2_pdr_leiden_f4.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_f4.H2c" "H2"
#
#
# h2_pdr_leiden_f4.in
# class pdr
# ======================================
#
```

---

h2_pdr_leiden_hack_f1.in

low density low flux model 1 as defined in e-mail

```
title low density low flux model 1 as defined in e-mail
database h2
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16
#
# commands controlling geometry =========
#
```

```
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "h2_pdr_leiden_hack_f1.per"
save leiden lines "h2_pdr_leiden_hack_f1.lin"
save leiden "h2_pdr_leiden_hack_f1.lei"
save dr "h2_pdr_leiden_hack_f1.dr"
save grain physical conditions "h2_pdr_leiden_hack_f1.grn"
save overview "h2_pdr_leiden_hack_f1.ovr"
#
save H2 lines "h2_pdr_leiden_hack_f1.h2lin"
save H2 column density "h2_pdr_leiden_hack_f1.h2col"
save H2 populations "h2_pdr_leiden_hack_f1.pop"
save H2 populations zone "h2_pdr_leiden_hack_f1.zon"
save H2 populations matrix "h2_pdr_leiden_hack_f1.mat"
#
# h2_pdr_leiden_hack_f1.in
# class pdr
# ========================================
#
```

---

h2_pdr_leiden_v1.in

model 5 as defined in e-mail

```
title model 5 as defined in e-mail
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# is half the requested value
# they want for the model is actually twice the value below
table draine 5
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
# add PAHs
grains PAH no qheat 3 function
database h2
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "h2_pdr_leiden_v1.per"
save overview "h2_pdr_leiden_v1.ovr"
save leiden lines "h2_pdr_leiden_v1.lin"
save leiden "h2_pdr_leiden_v1.lei"
save dr "h2_pdr_leiden_v1.dr"
save grain dust temperature "h2_pdr_leiden_v1.grn"
save chemistry rates destruction "h2_pdr_leiden_v1.H2d" "H2"
```

```
save chemistry rates creation "h2_pdr_leiden_v1.H2c" "H2"
#
#
#
#
# h2_pdr_leiden_v1.in
# class pdr
# ======================================
#
```

---

h2_pdr_leiden_v2.in

model 6 as defined in e-mail

```
title model 6 as defined in e-mail
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
database h2
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "h2_pdr_leiden_v2.per"
save overview "h2_pdr_leiden_v2.ovr"
save leiden lines "h2_pdr_leiden_v2.lin"
save leiden "h2_pdr_leiden_v2.lei"
save dr "h2_pdr_leiden_v2.dr"
save grain dust temperature "h2_pdr_leiden_v2.grn"
save chemistry rates destruction "h2_pdr_leiden_v2.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_v2.H2c" "H2"
#
#
# h2_pdr_leiden_v2.in
# class pdr
# ======================================
#
```

---

h2_pdr_leiden_v3.in

model 7 as defined in e-mail

```
title model 7 as defined in e-mail
#
# commands controlling continuum =========
```

```
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
database h2
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "h2_pdr_leiden_v3.per"
save overview "h2_pdr_leiden_v3.ovr"
save leiden lines "h2_pdr_leiden_v3.lin"
save leiden "h2_pdr_leiden_v3.lei"
save dr "h2_pdr_leiden_v3.dr"
save grain dust temperature "h2_pdr_leiden_v3.grn"
save heating "h2_pdr_leiden_v3.het"
save cooling "h2_pdr_leiden_v3.col"
save molecules "h2_pdr_leiden_v3.mol"
save chemistry rates destruction "h2_pdr_leiden_v3.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_v3.H2c" "H2"
#
#
# h2_pdr_leiden_v3.in
# class pdr
# ========================================
#
```

---

h2_pdr_leiden_v4.in

model 8 as defined in e-mail

```
title model 8 as defined in e-mail
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
# insure that no H-ionizing radiation strikes cloud
extinguish 24
#
# commands for density & abundances =========
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
```

```
init file="pdr_leiden.ini"
database h2
#
# commands controlling output =========
save performance "h2_pdr_leiden_v4.per"
save overview "h2_pdr_leiden_v4.ovr"
save leiden lines "h2_pdr_leiden_v4.lin"
save leiden "h2_pdr_leiden_v4.lei"
save dr "h2_pdr_leiden_v4.dr"
save grain dust temperature "h2_pdr_leiden_v4.grn"
save chemistry rates destruction "h2_pdr_leiden_v4.H2d" "H2"
save chemistry rates creation "h2_pdr_leiden_v4.H2c" "H2"
save heating "h2_pdr_leiden_v4.het"
save cooling "h2_pdr_leiden_v4.col"
save h2 cool "h2_pdr_leiden_v4.h2col"
#
#
# h2_pdr_leiden_v4.in
# class pdr
# ======================================
#
```

---

h2_th85orion.in

Tielens and Hollenbach pdr model with orion grains, Table 2, paper b

```
title Tielens and Hollenbach pdr model with orion grains, Table 2, paper b
failures 3
#
print line sort intensity
print line column
iterate
#
# cosmic background
background
cosmic rays, background
#
set nend 2000
# simulate effects of gas we do not model
double
#
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t=75K
intensity 2.7 (total)
#
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
#
# this will remove all ionizing radiation
extinguish 24 0
#
hden 5.362
grains orion
grains PAH
database h2
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
turbulence 2.7 km/sec
normalize to "C 2" 157.636m
sphere
database H-like Lyman pumping off
cosmic rays, background
# this should be the one actually used
```

```
stop AV 33.2
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness so that would make results very
# detail dependent
stop thickness 19
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "h2_th85orion.per"
save overview last "h2_th85orion.ovr" no hash
save pdr last "h2_th85orion.pdr"
save molecules last "h2_th85orion.mol"
save dr "h2_th85orion.dr"
save hydrogen physical conditions last "h2_th85orion.hyd"
save results last "h2_th85orion.rlt"
save continuum units microns last "h2_th85orion.con"
save fine conti unit last micron "h2_th85orion_con.fin" range 0.09116 to 0.13 skip 2
save heating last "h2_th85orion.het"
save cooling last "h2_th85orion.col"
save hydrogen 21 cm last "h2_th85orion.21cm"
save chemistry rates destruction "h2_th85orion.H2d" "H2"
save chemistry rates creation "h2_th85orion.H2c" "H2"
#
#
# h2_th85orion.in
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR). Specifically, this is my attempt at their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

`m17_p07.in`

Pellegrini+07 2007ApJ...658.1119P model for M17

```
title Pellegrini+07 2007ApJ...658.1119P model for M17
# a brief description of its purpose
#
# commands controlling incident radiation field =========
# these give the shape and intensity
brems 8500000K
luminosity 33.5 range 7.35 to 176 Ryd
table star CoStar, 47490K
Q(h) 49.63
table star CoStar, 45335K
Q(h) 49.47
table star CoStar, 43151K
Q(h) 49.30
table star CoStar, 41209K
Q(h) 49.18
table star CoStar, 39084K
Q(h) 49.08
table star CoStar, 36982K
Q(h) 48.81
table star atlas, 34914K
Q(h) 48.97
table star atlas,27700K
```

```
absolute bolometric magnitude -8.5
table star atlas, 23700K
absolute bolometric magnitude -7.5
table star atlas, 20350K
absolute bolometric magnitude -6.6
table star atlas, 17050
absolute bolometric magnitude -6.3
CMB
#
# commands for density & abundances =========
hden 2.065
abundances H II region no qheat no grains
grains PAH 10
grains orion 1
element Helium abundance -0.98
element Carbon abundance -4.14
element Nitrogen abundance -4.2
element Oxygen abundance -3.47
element Neon abundance -4.4
element Sulphur abundance -5.06
element Chlorine abundance -6.88
element Argon abundance -5.64
element Iron abundance -5.5
# these are to speed things up a bit
element limit off -6.9
#
# commands controlling geometry =========
radius 0.35355 linear parsecs
# the observed extinction along this sight line
stop Av extended 6.36
# do not want to stop at too small a depth due to low temperature
stop temperature off
# magnetostatic equilibrium
constant pressure
sphere
#
# other commands for details =========
magnetic field tangled -4.3125 2
turbulence 3km/s
iterate
cosmic rays background 1.60
#
# commands controlling output =========
save performance "m17_p07.per"
save lines emissivity last "m17_p07.ems"
H 1 6562.80A
Blnd 6720
CO 1300.05m
CO 2600.05m
CO 866.727m
CO 371.549m
C 2 157.636m
c 1 370.269m
c 1 609.590m
o 1 63.1679m
O 1 145.495m
Si 2 34.8046m
end of line
print line sort wavelength
print line optical depths faint -100
save species last "m17_p07.oh" "OH[:]" densities
save overview last "m17_p07.ovr"
save hydrogen 21 CM last "m17_p07.h21"
save pressure last "m17_p07.pre"
save molecules last "m17_p07.mol"
save heating last "m17_p07.het"
save cooling last "m17_p07.col"
save continuum last "m17_p07.con" units microns
#
#
```

```
# m17_P07.in
# class hii pdr
# ======================================
#
```

This is the magnetostatic model of the M17 H+ / H0 / H2 region presented in Pellegrini et al. 2007, ApJ, 658, 1119

`orion_hii_pdr_pp.in`

the Orion HII Region / PDR / Molecular cloud with an open geometry

```
title the Orion HII Region / PDR / Molecular cloud with an open geometry
#
# commands controlling continuum =========
# the incident continuum has two parts
# kurucz continuum with flux of photons striking cloud
# this is the the OVI star, its temperature and phi(H)
# this is the result of this command
# table star kurucz 39600 K
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_kurucz_39600.dat"
phi(H) 13
#
# this adds the observed hot brems
# its temperature (as log of T) and the flux of
# photons striking the cloud
brems 6
phi(h) 10
#
# cosmic rays are important for pdr chemistry
cosmic rays, background
#
# commands controlling geometry =========
# this turns off the stop temperature option
# so the sim will not stop due to temperature
stop temperature off
# this sets the thickness of the HII region & PDR
stop thickness 0.5 linear parsec
# this is typical of a gmc, larson 1981
# stop total hydrogen column density 22
# this will result in a milli gauss B-field in molecular region
magnetic field -5 gauss
# assume constant pressure
constant pressure
set nend 2500
#
# other commands for details =========
failures 3
# mimic existence of unmodeled molecular gas
double
# iterate since lines optically thick
iterate
# set microturbulence in equipartition with B field
turbulence equipartition
# set the line width so lines appear on the save continuum
# set save line width 10 km/s
#
# commands for density & abundances =========
# this is the log of the initial H density, cm-3
hden 4
# this will speed up the calculation a bit
init file="ism.ini"
# this uses HII region abundances, but no grains
abundances hii region no grains
```

```
# this uses orion grains
grains orion
# turn on PAHs, with an abundance that depends on H0 fraction,
# as suggested by long-slit observations of Orion bar,
# with an abundance 3x larger than default built into the code
grains pah function 3
#
# commands controlling output =========
# print lots of faint CO lines
print line faint -6
# normalize to Ha
normalize to "H 1" 6562.80A
save performance "orion_hii_pdr_pp.per"
save overview last "orion_hii_pdr_pp.ovr"
save temperature last "orion_hii_pdr_pp.tem"
save overview "orion_hii_pdr_pp.ovr1"
save molecules last "orion_hii_pdr_pp.mol"
save molecules "orion_hii_pdr_pp.mol1"
save heating "orion_hii_pdr_pp.het"
save cooling "orion_hii_pdr_pp.col"
save dr last "orion_hii_pdr_pp.dr"
save results last "orion_hii_pdr_pp.rlt"
save continuum last "orion_hii_pdr_pp.con" units microns
save hydrogen 21 cm last "orion_hii_pdr_pp.21cm"
save hydrogen lya last "orion_hii_pdr_pp.lya"
save element silicon last "orion_hii_pdr_pp.sil"
save pressure last "orion_hii_pdr_pp.pre"
save pressure "orion_hii_pdr_pp.pre1"
save grain extinction last "orion_hii_pdr_pp.grnext"
save grain charge last "orion_hii_pdr_pp.grnchr"
save grain potential last "orion_hii_pdr_pp.grnpot"
save grain temperature last "orion_hii_pdr_pp.grntem"
save grain temperature "orion_hii_pdr_pp.grntem1"
#
#
# orion_hii_pdr_pp.in
# class hii pdr
# ========================================
```

Similar to orion_hii_pdr except for plane parallel geometry. The properties of the molecular region change when details of the H+ region change because the pressure of the entire cloud can change as a result. The goal of this sim is an existence proof - that it can be done, rather than the stable details of the molecular region.

`pdr_xdr.in`

XDR sim

```
title XDR sim
CMB
ionization parameter -2.5
AGN 6.00 -1.40 -0.5 -1.0
extinguish 23
hden 3.5
abundances ism
grains PAH 3
stop H2 column density 22.0
sphere
stop temperature linear 3
normalize to "C 2" 157.636m
iterate
Database H-like Lyman pumping off
cosmic ray rate -16.3
save performance "pdr_xdr.per"
save overview "pdr_xdr.ovr"
save leiden "pdr_xdr.leiden"
```

```
save dr "pdr_xdr.dr"
#
# pdr_xdr.in
# class pdr
# ======================================
#
```

This is an XDR sim proposed by Nick Abel

`time_cool_cp.in`

constant pressure cooling cloud

```
title constant pressure cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
constant pressure reset
# >> chng 20 oct 05, from -6 to -5 for load balancing
element limit off -5
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 400
stop time when temperature falls below 1e4 K
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cp"
save time dependent ".tim" no hash
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
#
# time_cool_cp.in
# class dynamics
# ======================================
#
```

test time dependent cooling at constant pressure

`time_cool_cp_eq.in`

constant pressure equilibrium cooling cloud

```
title constant pressure equilibrium cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
constant pressure reset
# >> chng 20 oct 05, from -6 to -5 for load balancing
element limit off -5
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 400
stop time when temperature falls below 1e4 K
# this will do equilibrium cooling
set dynamics populations equilibrium
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cp_eq"
save time dependent ".tim" no hash
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
#
# time_cool_cp.in
# class dynamics
# ========================================
#
```

test time dependent cooling at constant pressure

D.5 Sample Programs

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