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
