Hands-on session

*You should have downloaded all simulations
*You should have downloaded extra python scripts

If you can’t run the code, extract the tarball of simulations in ~/3DPDR/sims/
Add the python scripts in ~/3DPDR/plots/

Running a model with 3D-PDR

```
==========================|************************
3DPDR input parameters file|    ~~~ COMMENTS ~~~
==========================|------------------------
ics                       !Initial conditions directory
sims                      !Output directory
1Dn20.dat                 !Input file (20 char. max.)
test                      !Output file (20 char. max)
0                         !HEALPix level of refinement
1.3                       !Theta critical (0<phi<pi/2)
8                         !First set of Chemical Iterations
6000                      !Total iterations
0.0                       !min number density (cm^-3)
1e12                      !max number density (cm^-3)
1e-17                     !Cosmic Rays (s^-1)
1.0                       !Turbulent velocity (km/s)
20.0                      !Dust temperature (K)
1e7                       !End time (yr)
100.0                     !Gas-to-dust
1.0                       !Metallicity
0.42                      !Omega
1.0E-5                    !Grain radius (cm)
==========================|
Input files for molecules  |*** 20 characters max ***
==========================|
12co.dat                  !CO
12c+.dat                  !CII
12c.dat                   !CI
16o.dat                   !OI
==========================|
Thermal balance values     |
==========================|
40.0                      !Initial temperature (used when TEMP_GUESS is OFF)
10.0                      !Tlow (used when TEMP_GUESS is OFF)
8000.0                    !Thigh (used when TEMP_GUESS is OFF)
10.0                      !Tmin (absolute lower bound)
100000.0                  !Tmax (absolute upper bound)
0.005                     !Fcrit (% Accuracy)
0.01                      !Tdiff (maximum temperature difference)
==========================|
UV field                  |
==========================|
UNI                       !ISO-tropic, UNI-directional
1                         !G0 (in Draine field units) -x t[illegible]x in 1D
```

Initial conditions

Output prefix

Cosmic-ray ionization rate

Metallicity

FUV intensity (Draine)

params.dat
This in the ~/3DPDR/ directory

Running a small grid of models

For all simulations, please use the n=1000 cm^{-3} density (**1Dn30.dat**)

PREFIX	CR (ζ_{CR})	FUV (χ/χ_0)	Metallicity (Z)
SIM01	1e-17	1	1
SIM02	1e-17	1000	1
SIM03	1e-14	1	1
SIM04	1e-14	1000	1

Plotting the results

In the directory ~/3DPDR/plots/ type:

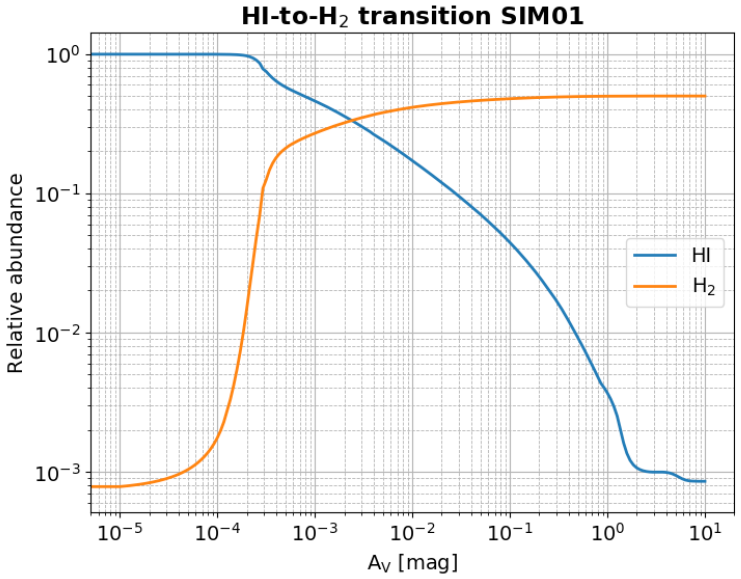
python profile.py SIMULATION_PREFIX

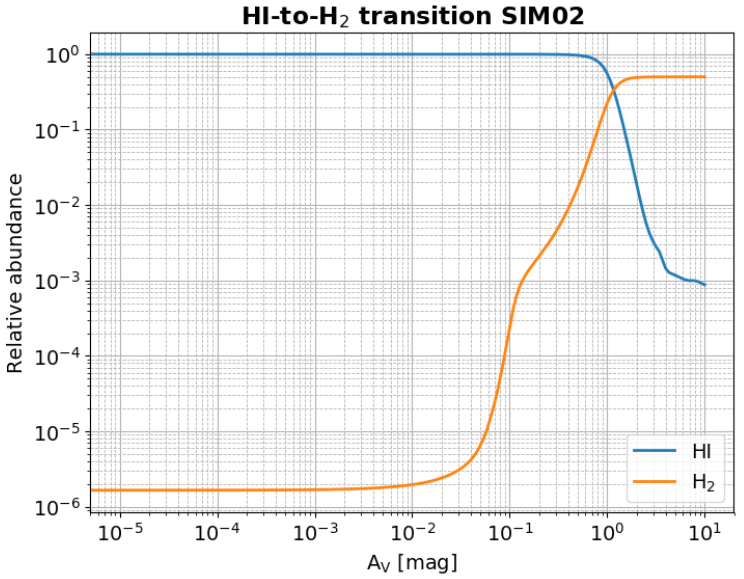
Question 1: find at what visual extinction, the HI-to-H2 transition occurs and also the CII / CI / CO transitions.

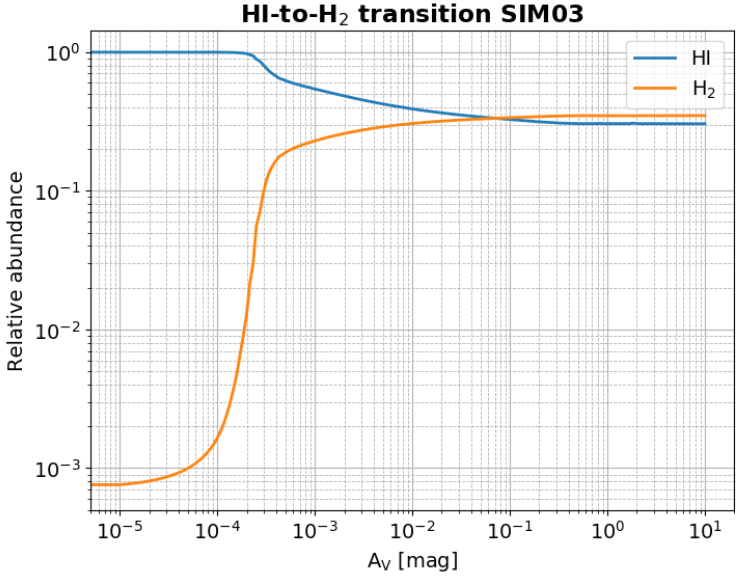
Question 2: Which environmental parameter(s) produce more molecular gas? Which produce more CO?

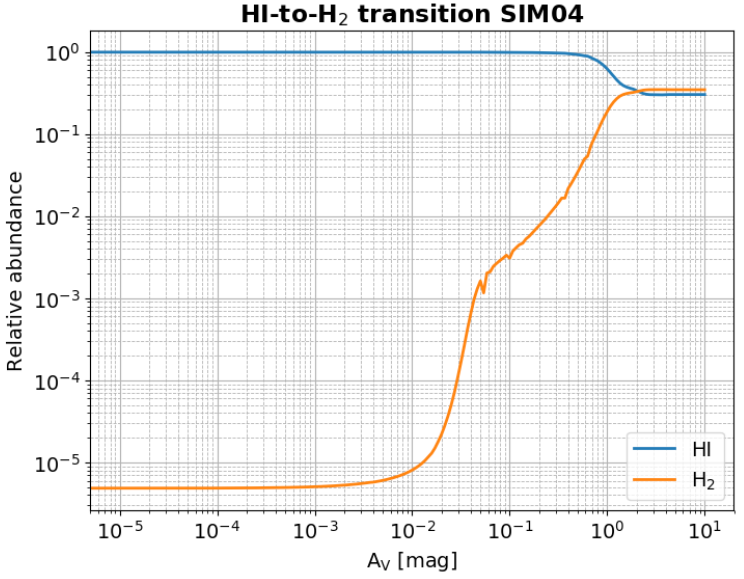
Question 3: Which environmental parameter(s) affect the gas temperature at low Av and which at high Av?

Plots for Q1-3

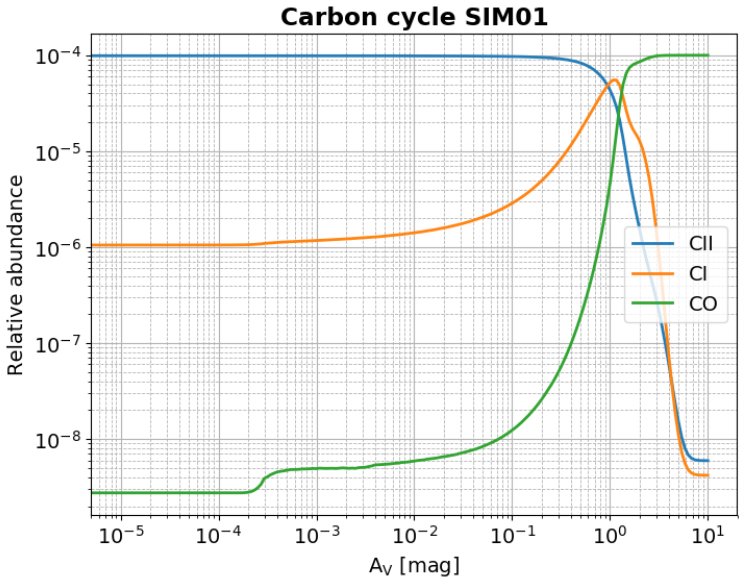


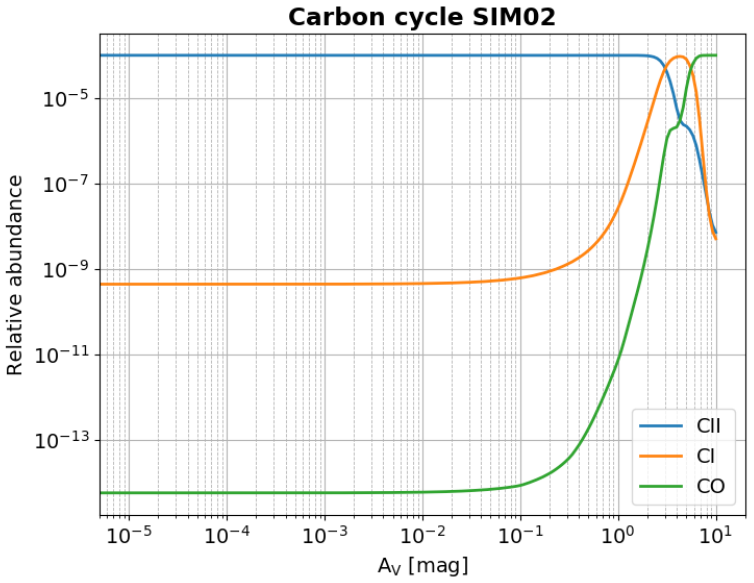


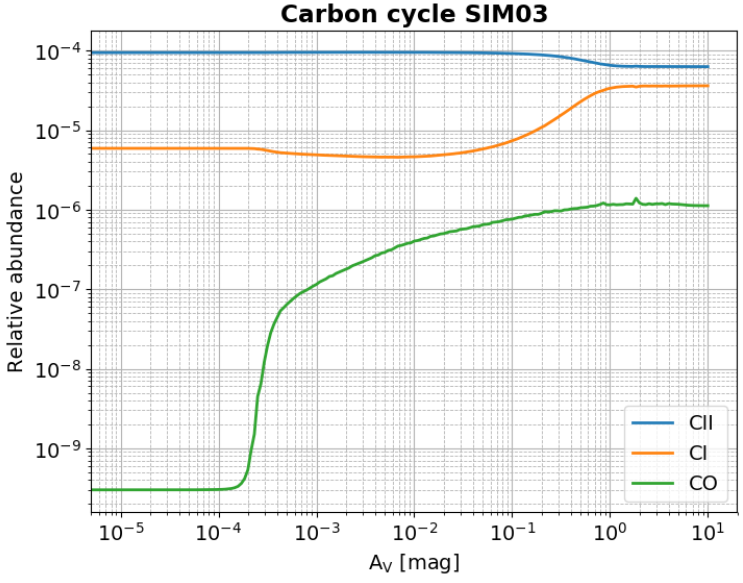


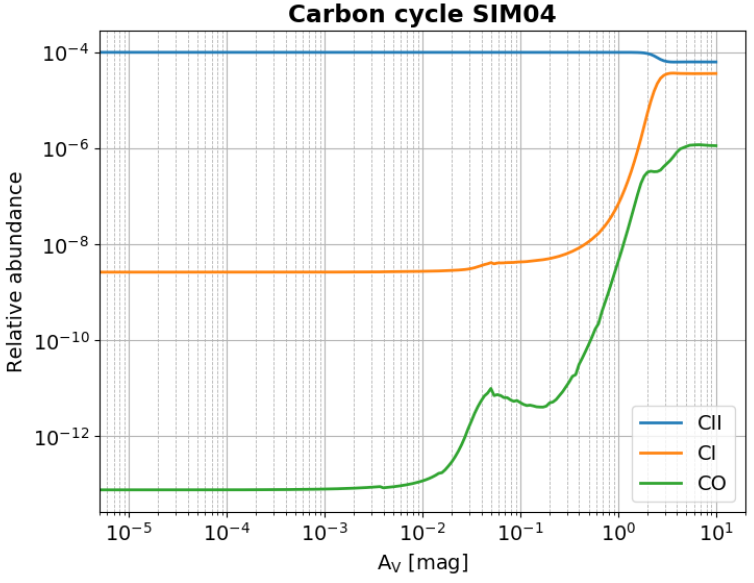


Plots for Q1-3

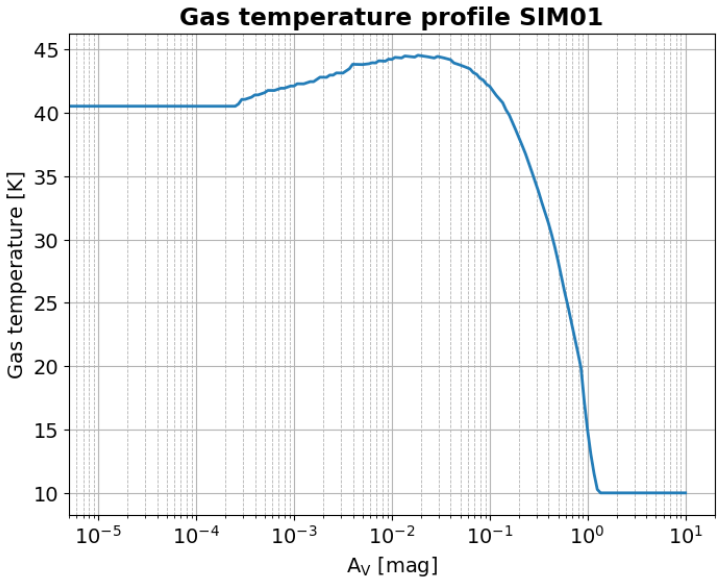


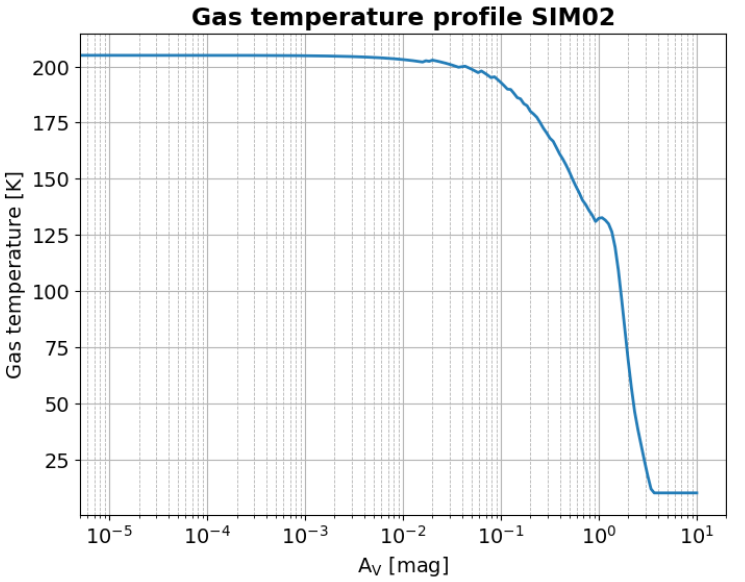


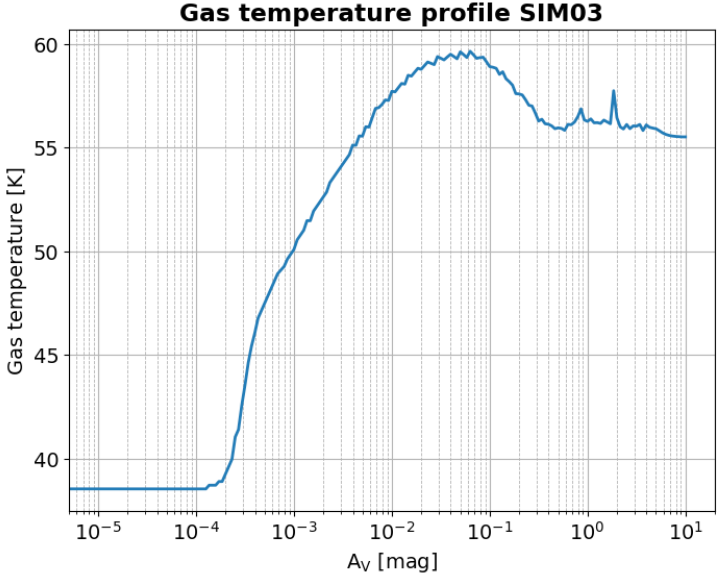


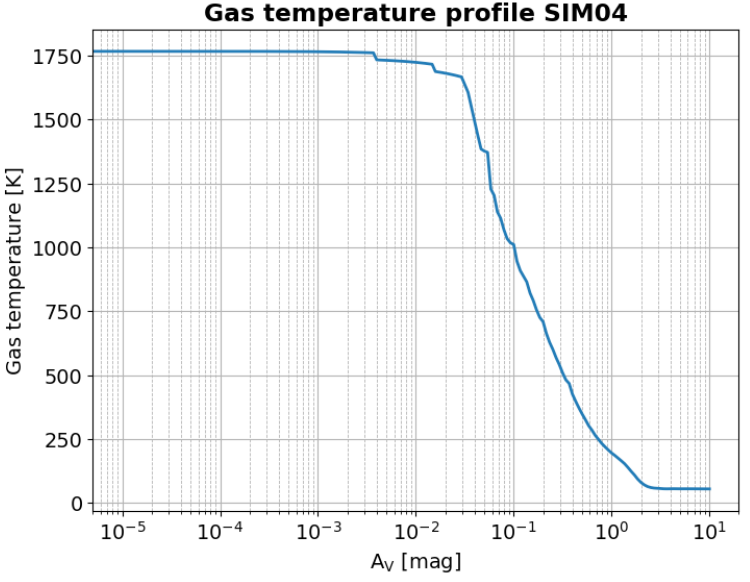


Plots for Q1-3









Plotting the results

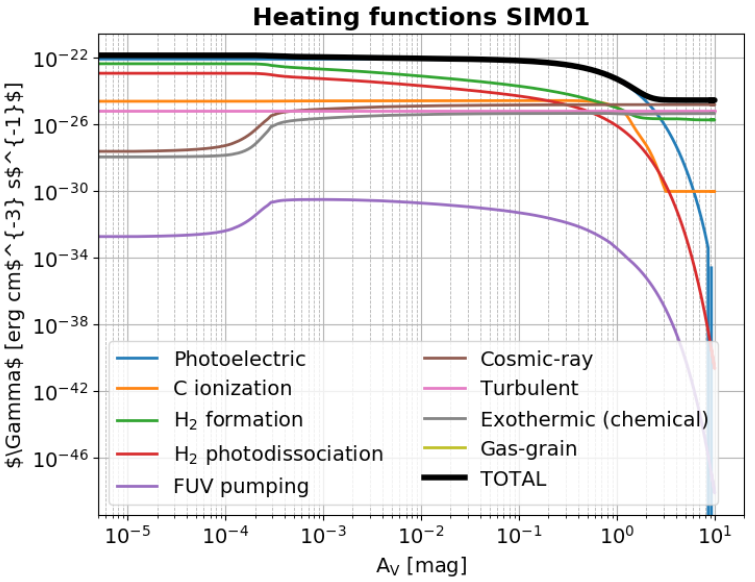
In the directory ~/3DPDR/plots/ type:

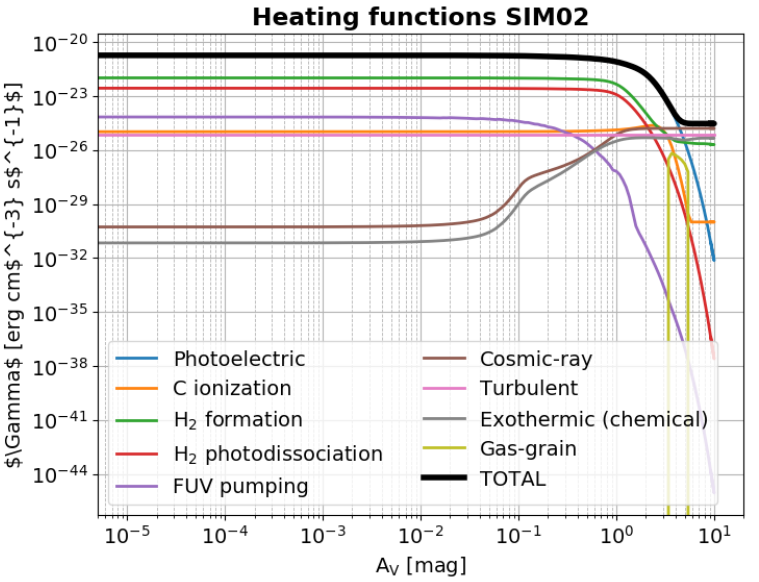
python hc_functions.py SIMULATION_PREFIX

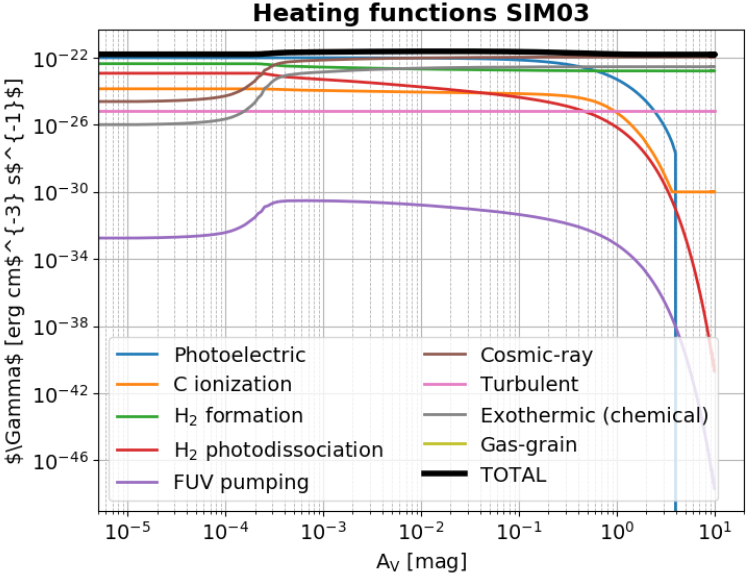
Question 4: Find the dominant heating mechanisms for each simulation as a function of Av

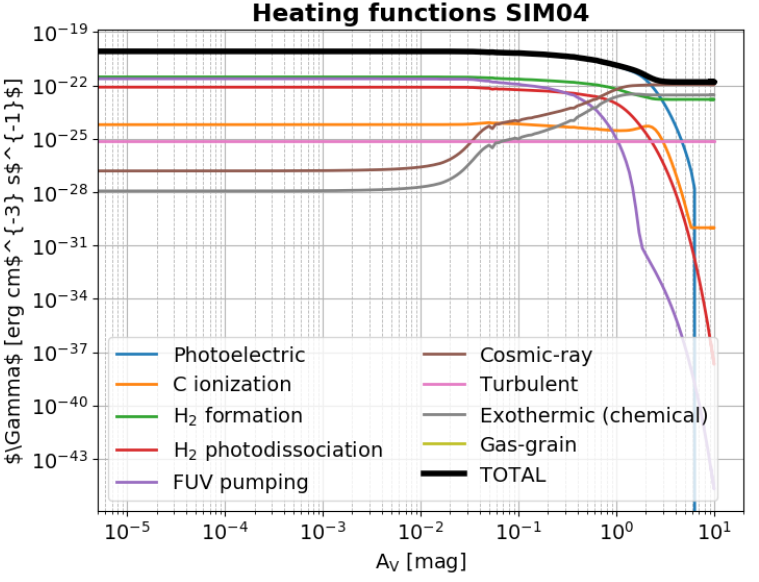
Question 5: Find the dominant cooling mechanisms for each simulation as a function of Av

Plots for Q4-5

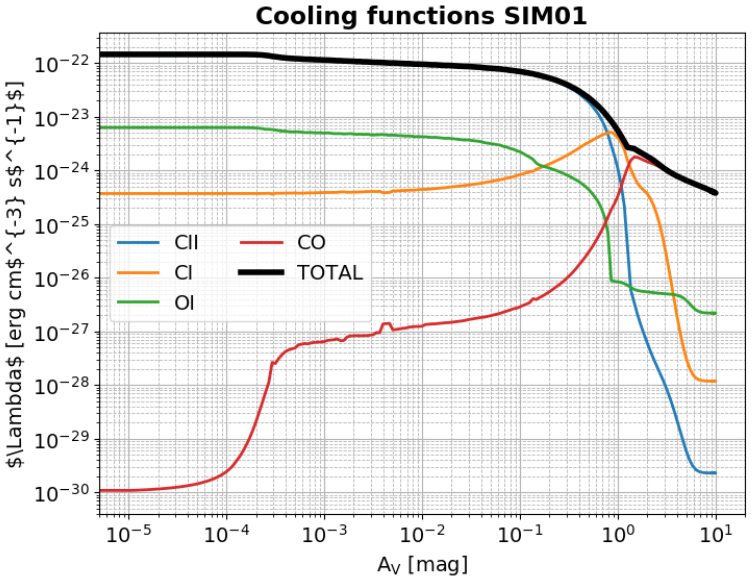


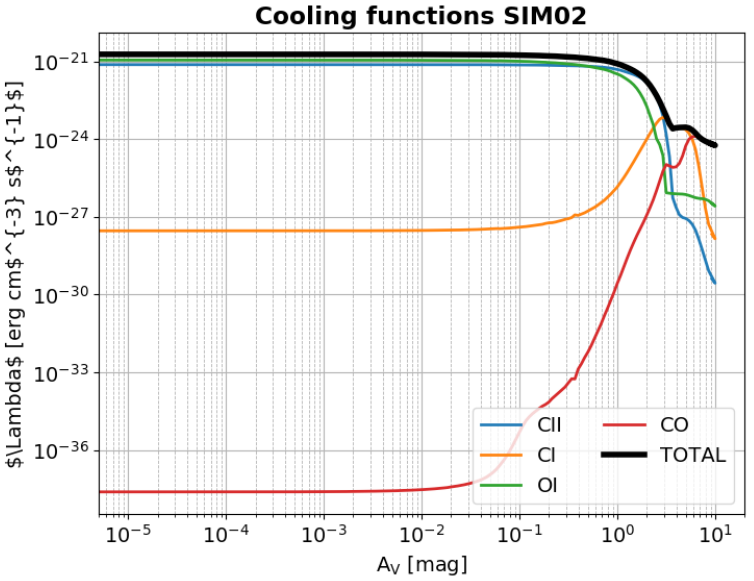


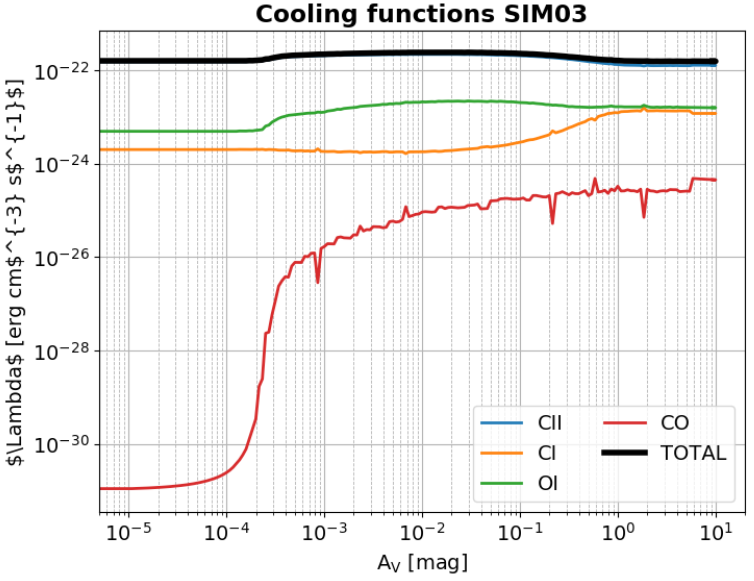


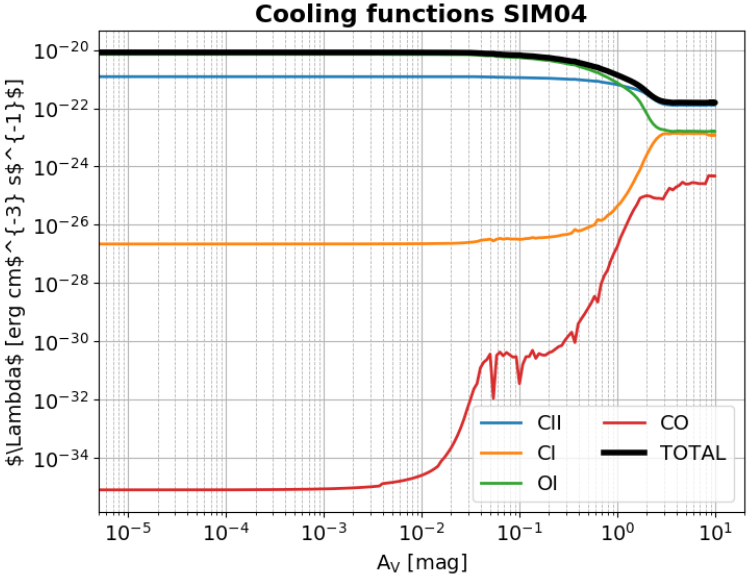


Plots for Q4-5







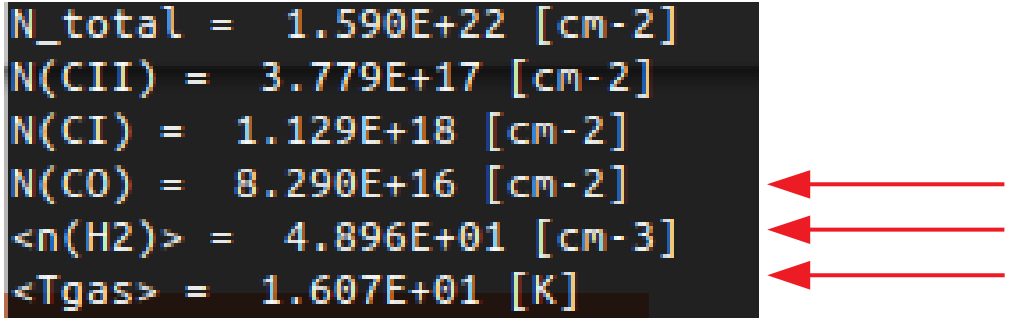


Constructing CO SLEDs

Step 1: Calculate a) CO column density, b) average H_2 number density, c) average gas (kinetic) temperature. To do this, use the columndensity.py script:

python columndensity.py SIMULATION_PREFIX

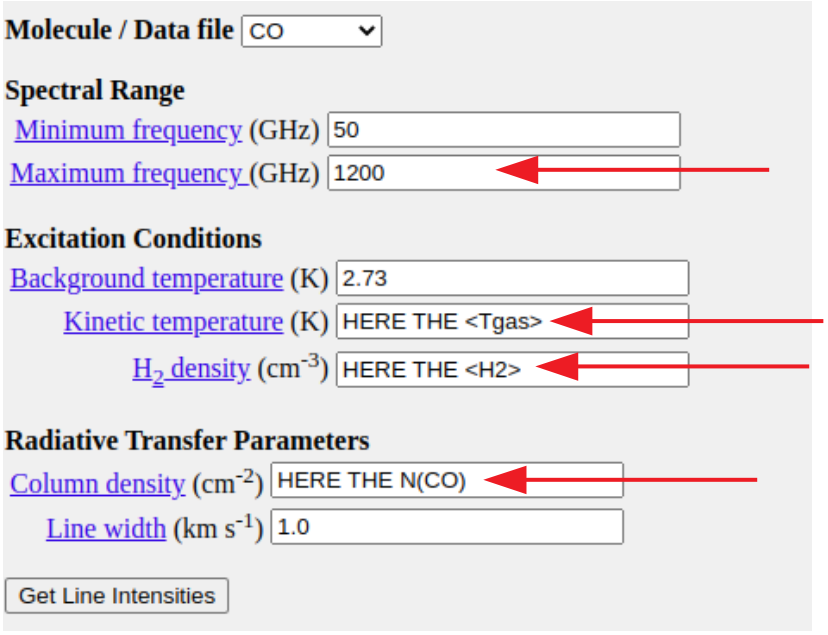
It should produce an output of the form:



RADEX (online, interactive)
http://var.sron.nl/radex/radex.php

Constructing CO SLEDs

Step 2: Insert the above quantities (a, b, c) in the RADEX online tool

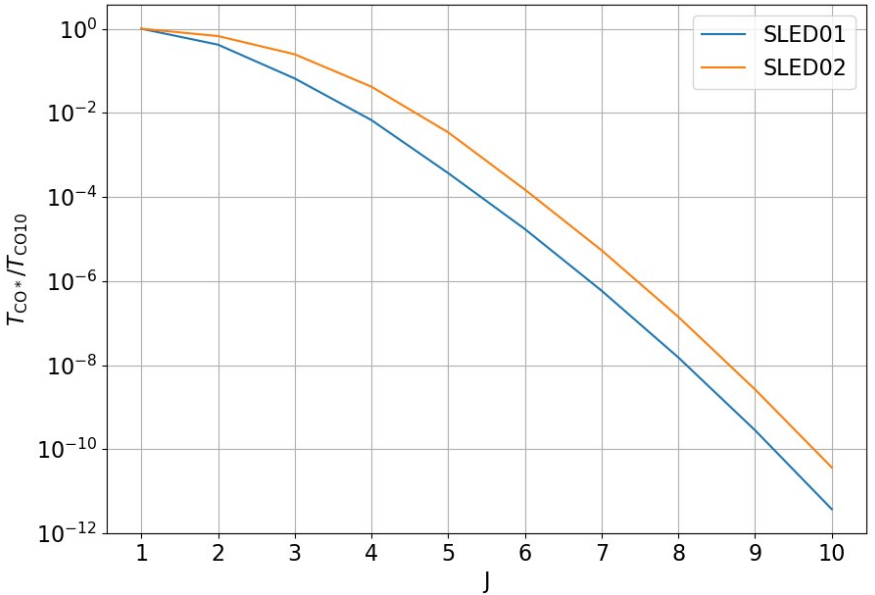


Transition	Frequency (GHz)	T_{ex} (K)	tau	T_R (K)
1 -- 0	115.2712	54.863	1.824E-03	9.349E-02
2 -- 1	230.5380	18.186	1.566E-02	2.023E-01
3 -- 2	345.7960	13.554	1.979E-02	1.347E-01
4 -- 3	461.0408	13.127	8.934E-03	4.471E-02
5 -- 4	576.2679	13.864	2.191E-03	9.526E-03
6 -- 5	691.4731	15.026	3.676E-04	1.505E-03
7 -- 6	806.6518	16.371	4.783E-05	1.921E-04
8 -- 7	921.7997	17.626	5.193E-06	2.032E-05
9 -- 8	1036.9124	18.587	4.796E-07	1.762E-06
10 -- 9	1151.9855	19.637	3.682E-08	1.297E-07

Copy what you see (as you see it) in a file called SLED01, SLED02 etc.

Constructing CO SLEDs

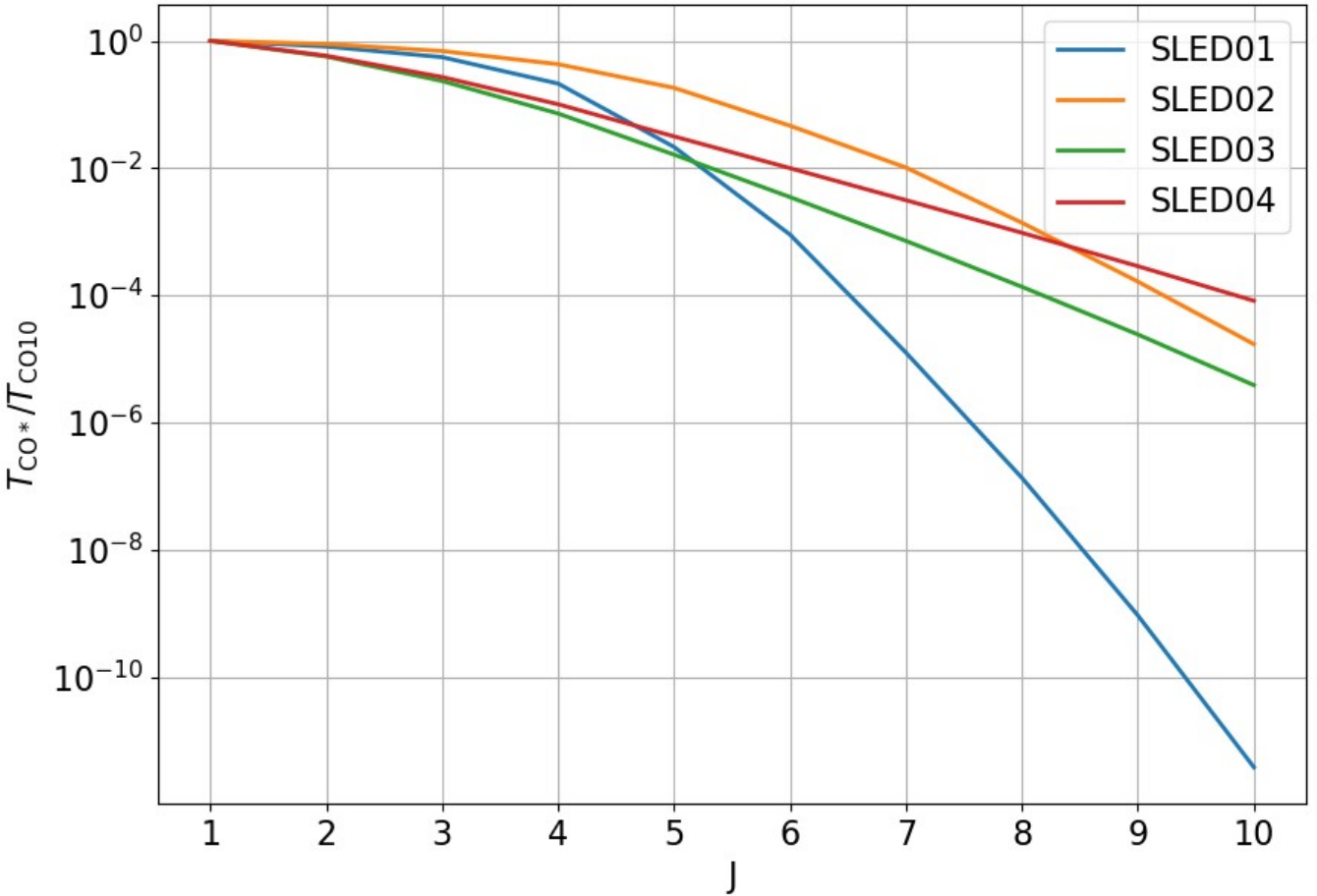
Type: python sled.py SLED01 SLED02
It should produce a diagram like the one below



Question 5: How do N(CI) and N(CO) change between SIM01-04? Which produces most of CI and which most of CO?

Question 6: How do CO SLEDs vary in SIM01-04?

Answers to column densities and CO SLEDs



Most of N(CI): SIM03
Most of N(CO): SIM01