

Manual for c3.4 Head File "physics_coeff.h"

In short:

	Related option
Number of levels	LEVEL_N
LVG Model	OneD, TwoD, Isotropic, Mix
C/A ratio, density of the collisional partner	NC
Viewing Angle	OBS_ANG
Temperature	TEMP_SELE
Molecule type	MOLE_DATA
Number of calculation points	TAU_N

Detail:

1. Output File Name Options

```
#define OUTPUT_VER "c3.4"  
#define OUTPUT_FILE_TAG "co"  
#define OUTPUT_TYPE ".csv"
```

The output file will be in the form of

OUTPUT_VER[LEVEL_N][Dim][NC NC][OBS_ANG PI][T K]OUTPUT_FILE_TAG+OUTPUT_TYPE

For example, if OUTPUT_VER = "c3.4", LEVEL_N = 5, TwoD = 1, NC = 2.1827273E+03, OBS_ANG = 0.5*M_PI, T = 30, OUTPUT_FILE_TAG = "co" and OUTPUT_TYPE = ".csv", then the file name will be:
c3.4[5][2D][NC 2.1827E3][0.5PI][30K]co.csv

2. GNUPlot file Output Option

```
#define GNUPLOT OUTPUT 1
```

It decides whether to generate GNUPlot file and data or not. (0: No, 1: Yes)

The GNUPlot data file name will be in the form of

OUTPUT_VER[LEVEL_N][Dim][NC NC][OBS_ANG PI][T K]OUTPUT_FILE_TAG.dat

The GNUPlot command file name will be in the form of

OUTPUT_VER[LEVEL_N][Dim][NC NC][OBS_ANG PI][T K]OUTPUT_FILE_TAG.dem

3. Molecule data file from LAMDA

```
#define MOLE_DATA "co.win.dat"
```

This is the file name of the molecule data file which contains the Einstein coefficients, collisional coefficients and energy level information.

For SiO, use "sio.win.dat".

The molecule data file should be located at the same directory as the program when you execute it.

4. Density of Molecule

```
#define Nt ((LEVEL_N+1)*LEVEL_N)/2
```

The density or the number of molecules in this cell. This option will not change the results of the program.

You can also use 1.0 instead.

```
#define NC 2.1827273E+03
```

This is the density of the collisional partner (in unit of cm⁻³). It decides the collisional coefficients and also the C to A ratio.

5. Velocity Gradient Model Options

```
#define OneD 0  
#define TwoD 1  
#define Isotropic 0  
#define Mix 0 //Mix of OneD and TwoD:
```

```
#define MixRatio 0.1 //MixRatio*sin^2 + cos^2
```

It decides the LVG Model. 0 for disable, 1 for enable. Choose only one model at a time.

OneD stands for one-dimensional velocity gradient.

TwoD stands for two-dimensional velocity gradient.

Mix stands for the mix model of one and two-dimensional velocity gradient, and the MixRatio decides the ratio.

Isotropic stands for isotropic case.

6. Viewing Angle Options

```
#if OneD ← Do not change this.
#define OBS_ANG 0.49167*M_PI
#define TAU_ANG OBS_ANG
#define TAU_START 0.001
#else
#define OBS_ANG 0.5*M_PI
#define TAU_ANG OBS_ANG
#define TAU_START 0.01
#endif
```

OBS_ANG decides the angle between the line of sight and the z axis.

TAU_ANG decides the angle between the z axis and the line which be used as the unit of TAU. It usually is set to OBS_ANG.

TAU_START decides the starting TAU of the calculation.

The options between #if OneD and #else are for one-dimensional case. The options between #else and #endif are for other cases.

7. TAU Region Options

```
#define TAU_N 151 //number of points in the curve
#define TAU_INC_RATIO 1.09647819614318 //optical depth increase ratio
```

They decide the points of optical depth which the calculation will be carried out at.

8. Number of levels

```
#define LEVEL_N 5
#define TOTAL_N ((LEVEL_N+1)*LEVEL_N)/2
#define TRANS_N ((LEVEL_N-1)*LEVEL_N)/2
```

LEVEL_N decides the number of levels. For example, if LEVEL_N = 5, then levels J = 0 ~ 4 will be included in calculation.

Do not change TOTAL_N and TRANS_N.

9. Temperature Options

```
#define TEMP_SELE 4
#define TEMP_B 2.725
```

TEMP_SELE decides which temperature option should be chose as the temperature of the cloud from the molecule data file.

TEMP_B is the cosmic blackbody radiation temperature (K).

10. Constant

```
#define h_CONST 6.62606896E-34 //Plank constant
#define LIGHT_SPEED 299792458.0 //Speed of light
#define k_CONST 1.3806504E-23 //Boltzmann constant
```

It takes the value from Wikipedia.

11. Convergent Options

```
#define REL_PREC 1E-6
#define EpsRel 1e-4
```

```
#define EpsAbs 0
```

REL_PREC is the criterion for iteration subroutine to decide whether the value of $n[]$ converges or not in each main loop.

EpsRel and EpsAbs decide the precision of integration for GSL integration subroutine.

12. Other Options

```
#define SLOW_MODE 0
```

```
#define Gsl_Integ_Space 3000
```

When SLOW_MODE is set to 1, the program will use thermal equilibrium population($n[]$) as the initial value in each main loop. Usually, it will not affect the results significantly.

Gsl_Integ_Space decides the memory space for GSL integration subroutine.

13. Debug Use Options

```
#define SHOW_A_V 0 //Show the A[] and v[] that read from MOLE_DATA
#define SHOW_C 0 //Show the C[] that read from MOLE_DATA
#define SHOW_NI 0 //Show the initial n[] that calculated by n_initial_cal()
#define SHOW_NF 0 //Show the final n[] that calculated by n_initial_cal()
#define OUTPUT_A_MATRIX_I 0 //Output the a_matrix_i[] that calculated by
a_matrix_initialize()
//and write it to the file A_MATRIX_I_FILE
#define A_MATRIX_I_FILE "a_matrix_i[].csv" //the output file of a_matrix_i[]
#define OUTPUT_E 0
#define E_FILE "E[].csv"
#define OUTPUT_BR_N 0
#define SHOW_BR_N 0
#define BR_N_FILE "Br_n[].csv"
```

These will not affect the results of calculation.

0: disable, 1: enable