

Project 98 : "What is the structure of the Circumstellar Gas around Massive Protostars?"  
Modeling the Molecular Emission from Young Protostars (CE, A)

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Quantum number for rotation :  $j!$  (Total angular momentum)

When does the assumption of a 'single temperature' model fail? What are the limitations?

$$\frac{^{12}\text{C}}{^{13}\text{C}} \approx 50 \text{ (in Solar System)} \text{ or } \approx 100 \text{ (interstellar)}$$

$$\text{but } \frac{\text{CH}_3\text{CN}}{\text{CH}_3^{13}\text{CN}} \neq 50$$

Workspace  $\Rightarrow$  across bridge in JBCA or ALMA room

NASA ADS

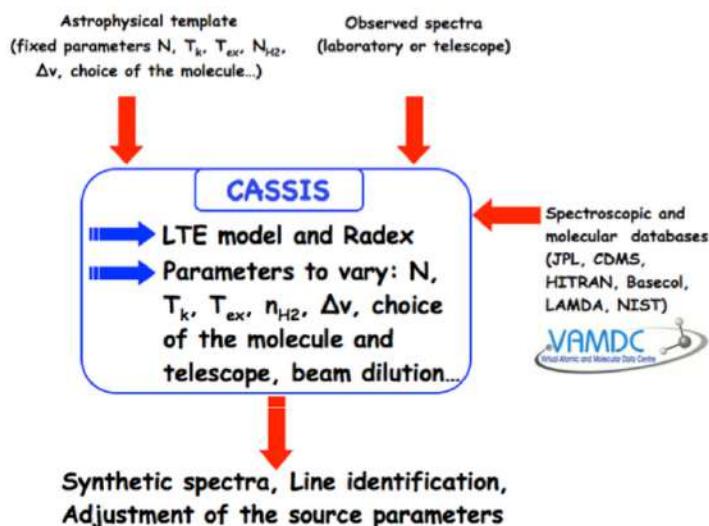
Zoom meeting Thursday?

Thursday 29/09/22

Began setting up computer environment using:

CASSIS - an interactive spectrum analyser

The current functionalities of CASSIS are:



7 parameters :

Column density

Line emission width

Excitation / Thermal energy

velocity

beam size?

temperature?

ALMA with 400m baseline

interferometer, 400m maximum separation  
 $\sim 0.67''$

Range of source lines

Need source-size larger than the beam  
or be 0.5 or 2x size

Velocity of source doesn't matter - can set as 0  
Line width does matter

"LTE model-2 comp.py" programme for creating  
LTE - local thermodynamic equilibrium model molecular emission spectra

04 / 10 / 22

Set up Gitkraken to keep a record of every change we make to the 'LTE-model' code, as we have to change parameters within the code.

Local repository at D:/university/year 4 / masters /  
physics repository  
(might need to move)



## Notes from '...hot cores in W43-MM1 ...'

- assumption that the source size is equal to the beam size

## Notes from 'Complex Organic Interstellar Molecules'

- Simulations of the chemistry provide a probe of the physical conditions in a protostar because the rates of ongoing reactions depend on said conditions

- isotopologues (molecules containing isotopes) do not in the same ratio as the isotope itself

Chemical fractionation, process by which chemical reactions produce abundance ratios among isotopologues different from the actual elemental abundance ratios.

In the absence of this chemical fractionation, the isotopologues can be used to determine elemental abundance ratios eg  $^{13}\text{C}/^{12}\text{C}$  at different places in the universe.

- Most interstellar and circumstellar molecules have been detected by their rotational spectral lines.



## Section 3

### Eq. 13 Single temperature excitation

Column density:

$$\frac{N_u}{g_u} = \frac{N_{\text{tot}}}{Q(T_{\text{rot}})} e^{-E_u/T_{\text{rot}}} = \frac{3k_B \int T_{\text{mb}} dV}{8\pi^3 \nu \mu^2 S}$$

where:  $N_u$  = total column density in the upper level;  
 $g_u$  = statistical weight of level  $u$ ;  
 $N$  = total column density of the molecule;  
 $k_B$  = Boltzmann const.;  
 $\nu$  = transition frequency;  
 $\mu$  = permanent dipole moment;  
 $S$  = intrinsic line strength;  
 $\int T_{\text{mb}} dV$  = measured integrated main beam density [ $\text{K} \cdot \text{km s}^{-1}$ ]

Hot core definition (vonder Tak, F.F.S, 2003):

- ☆ Column density  $N > 10^6 \text{ cm}^{-2}$
- ☆  $T > 100 \text{ K}$  (but  $< 500 \text{ K}$  (Encyclopedia of Astrobiology, Charley S., 2011))
- ☆ size:  $d < 0.1 \text{ pc}$

06/10/22

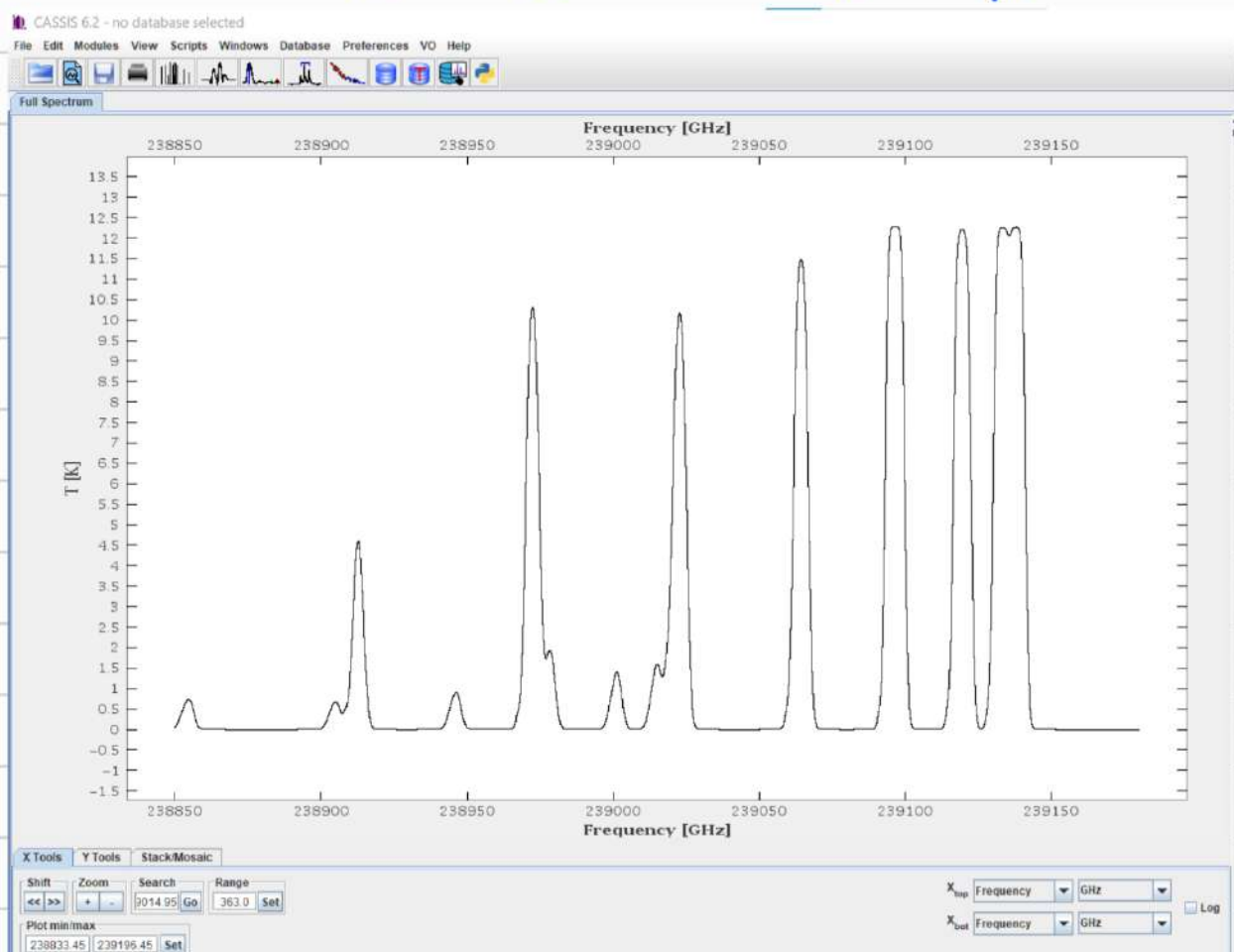
Run Python 'LTE-model' code to produce simulated emission line spectra of  $\text{CH}_3\text{CN}$

Within code, two molecules (isotopologues of each other) with ratio of 60.

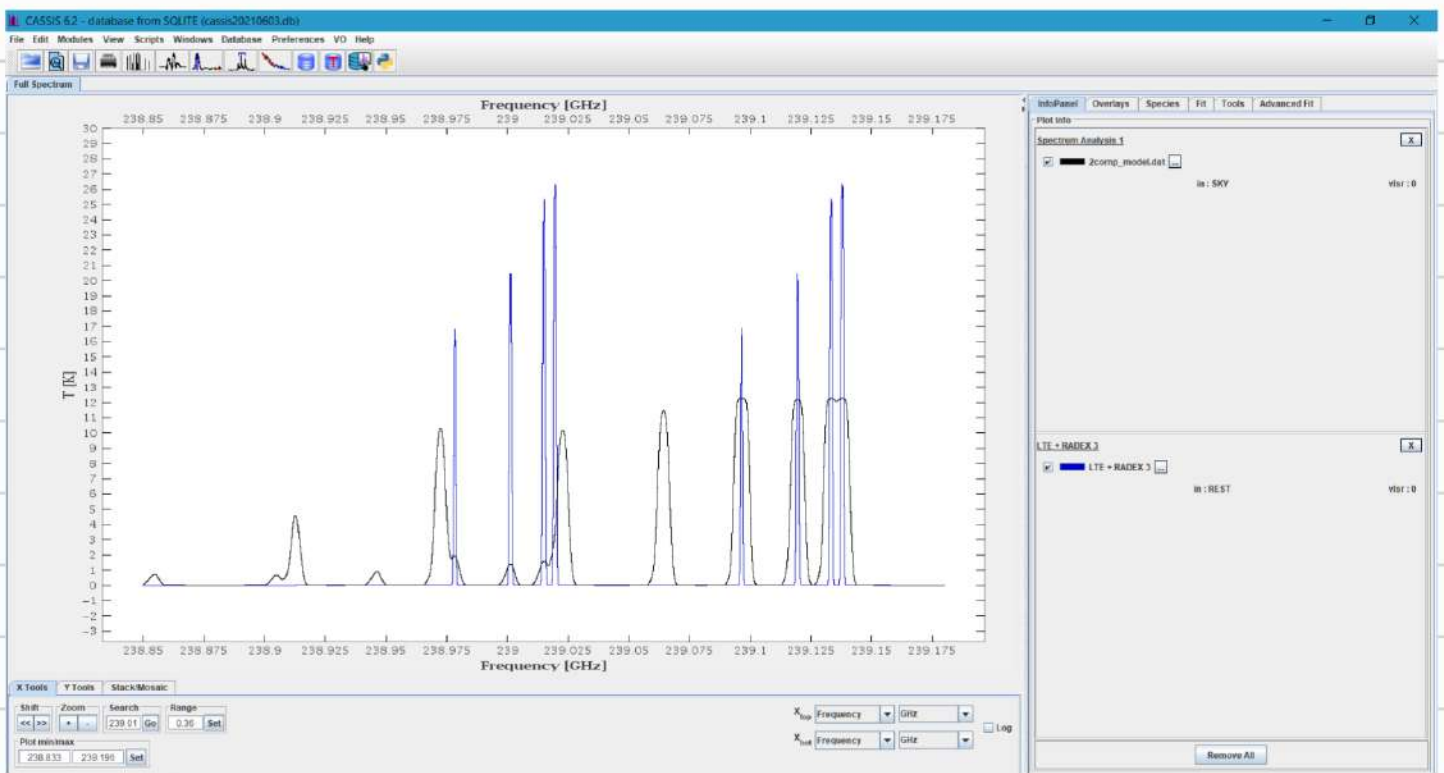
Parameters have array of upper and lower limits used to generate random values in between.

$\text{CH}_3\text{CN}$  has vibrational states  $\nu_1 \rightarrow \nu_8$   
(where  $\nu_1$  is the first excited state etc.)

Updated Java - fixed database access issue!  
Can now use LTE+RADEX fit







LTE + RADEX 3

Tuning

K Range: min: 238.85 max: 239.175 GHz dv: 0.1 MHz

Line: 111.5 Bandwidth: 8.0 GHz ☐ DSB ☐ LO freq: 12.1 Telescop: alma\_400m

Threshold

Etp: min: 0.0 max: 150.0 K ☐ A min: 0.0 max: Einstein coefficients

Jup min: max: K<sub>up</sub> min: max: K<sub>up</sub> min: max: K<sub>up</sub> min: max:

LTE+RADEX ☒

Telescop: alma\_400m ☐ Trib>Te\*

Observing Mode: PSWDBSw Background: Top: 2.73 K Noise: rms: 0.0 mK Frequency Scale: Best frequency

Confirmations ☒ Component 1 X

Model: Full LTE Species: All Species

Interacting Geometry: Spherical

N<sub>H2</sub> (cm<sup>-2</sup>): 7.5E22 V<sub>rot</sub>:

Name	Id	Database	Compute	N(S) (cm <sup>-2</sup> )	Abundance (H <sub>2</sub> )	Tex (K)	FWHM (km/s)	Size (")
CH3C13H	42007	JPL	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=0	42009	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=1	42010	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=2	42011	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=3	42012	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=4	42013	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=5	42014	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=6	42015	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=7	42016	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=8	42017	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=9	42018	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=10	42019	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=11	42020	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=12	42021	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=13	42022	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=16	42025	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=17	42026	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=18	42027	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=19	42028	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=20	42029	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=21	42030	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=52	42061	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=65	42074	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=69	42078	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=73	42082	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=74	42083	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
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CH3C13H v=97	42106	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=98	42107	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=99	42108	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00
CH3C13H v=100	42109	CDMS	<input checked="" type="checkbox"/>	7.00E14	8.33E-9	35.00	1.00	3.00

Load config Save config Help Display

initial fit was 'bad', looks like it doesn't account for spectral broadening?

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Boltzmann equation for two-level system

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\frac{E_2 - E_1}{k_B T}}$$

temperature  
is a characterisation of the  
state

LTE assumes temp. of gas (eg thermometer inserted) is the excitation temp.

$$\text{ie } T_k = T_g = T_{ex}$$

If using lowest two states, get exc. temp., next two states also give same exc. temp.

Could look if all energy levels are in LTE

FWHM velocity dispersion of molecules in the gas.

If gas purely thermal, vel. would be directly related to temp.

Reality is that there is an unresolved motion component (non-thermal) that we characterise by this FWHM (sets how 'wide' the line will be)



Small source with big beam, get all flux

Smaller beam than source, get fraction of flux

Planck bb function units of specific intensity

$$\text{flux} = \text{specific intensity} \times \text{solid angle}$$

$$\text{flux} = \int I_\nu d\Omega$$

Beam size smaller than source, line temperatures don't change with

$$\text{cd den} : 10^{14} \rightarrow 10^{17}$$

$$\text{exc. temp} : 20, 30\text{K} \rightarrow 300, 400\text{K}$$

$$\text{fwhm} : 2 \rightarrow 10$$

$$\text{source size} : 0.2 \rightarrow 1.0 \text{ arcsec}$$

Generate sets of spectra where one parameter is varied through a range whilst the rest are held fixed.

Gravy group seminar Thursday @ 3pm

Output dat files named according to their variable and stored in folders according to each varied range.

D:\UNIVERSITY\YEAR 4\MASTERS\mphys  
repository\mphys 1 dat files

then eg. \extemp

Variables held constant at

colden =  $1e15$

extemp = 200

fullwidth = 5

lsr\_vel = 0

source size = 0.7

iso ratio = 60

Following changes observed in both  $\text{CH}_3\text{CN}$  and  $\text{CH}_3^{13}\text{CN}$ :

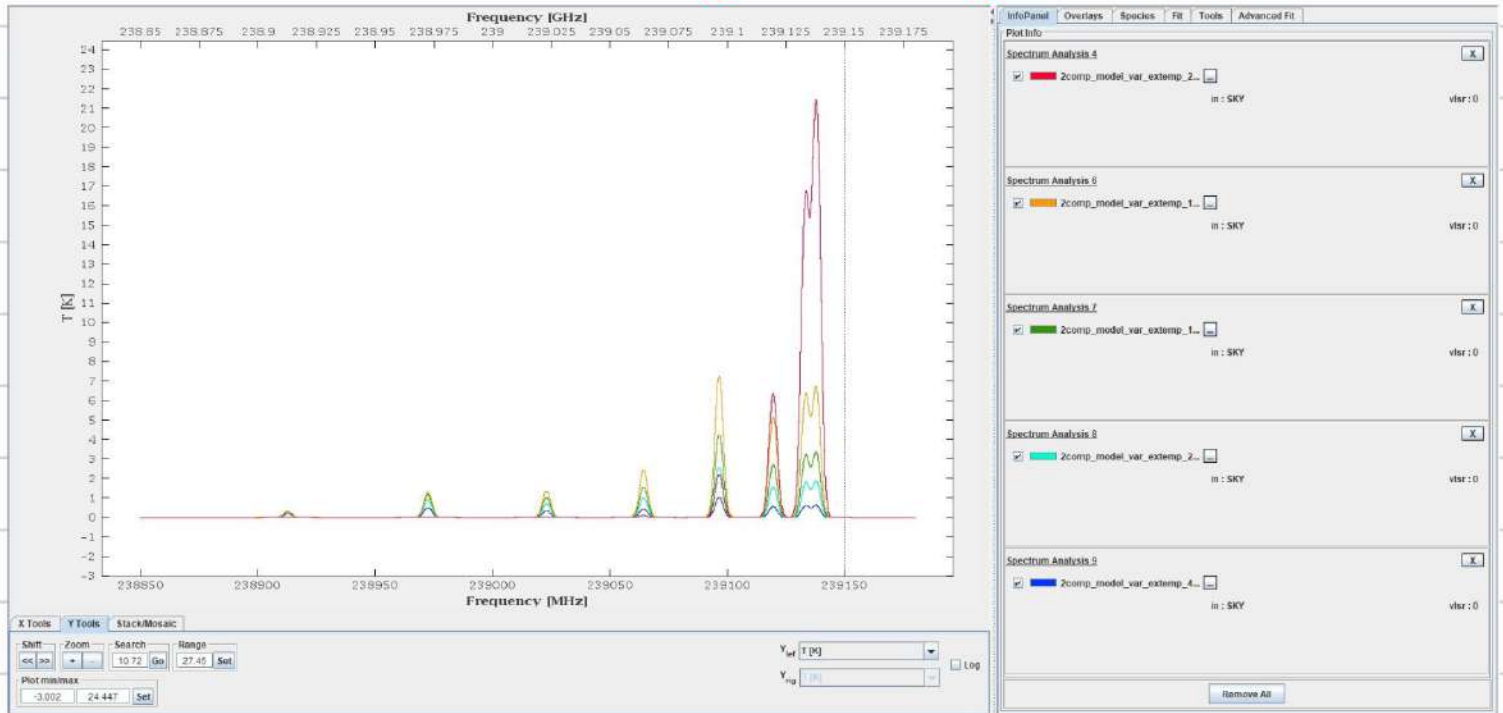
increasing 'colden': increasing peak height,  
there is more material present,  
more flux and so larger intensity  
(brightness temp.) detected

Eventually photons can't escape  
- saturate



increasing 'extemp': peaks seem to 'appear' at the left, and peak intensities decrease with higher frequencies impacted more.

Decreasing optical depth with increasing temp.  $\rightarrow$  decreasing intensity



increasing source size: increases the intensity, but the 'shape' stays the same.

ALMA (400m baseline)  
beam size  
(assuming  $f = 2.39 \times 10^{11}$  GHz)  
 $\Rightarrow \lambda = 1.25 \times 10^{-3}$  m

$$\theta = \frac{1.22 \lambda}{D} = 3.81 \times 10^{-6} \text{ rad} \quad \cdot \frac{3600 \times 180}{\pi}$$

$$= 0.789''$$

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Varying two parameters:

so far, our datasets are just varying one parameter and holding every other constant.

This approach, however, will fail to observe how parameters might depend on each other.

Attempt with varying both



# Meeting

## discussions of our findings

increasing 'colden': increasing peak height,  
there is more material present,  
more flux and so larger intensity  
(brightness temp.) detected

→ peak height's 'plateau' at high  
colden. because the gas becomes optically  
thick and photons can no longer escape.  
The medium has become optically thick.

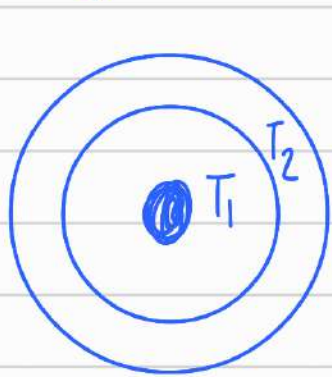
increasing 'extemp': peaks seem to 'appear'  
at the left, and peak intensities  
decrease with higher frequencies  
impacted more.

Peaks appear as more energy states become  
available, but overall intensity decreases  
because the increasing temperature decreases  
optical depth.

This was tested by numerically integrating  
to find the area beneath the spectrum.

Next:

use two components with different  
eg  $T_1$  and  $T_2$  (with  $\nu_{\text{rest}}$  held constant)



eg

$$T_2 < T_1$$
$$\delta_{T_2} > \delta_{T_1}$$

both of these  
regions are assumed  
to be in the beam

When saving combined (2-component) spectra,  
also save the two separate component  
spectra (ie end up with 3)

Jython : Java in Python

in examples, H2CO-MCMC

H2CO-RG-LTE



Week 4  
18/10/22

## Two component investigation

We will choose a parameter to vary whilst holding the rest constant.

To fully investigate the two components,  $\text{com}_1$  will be varied for three different values of  $\text{com}_2$ .

The combined spectra of the two components will then be analysed in CASSIS by making two separate fits - one with  $\text{com}_1$  and another with  $\text{com}_2$ .

Three spectra will be collected - for  $\text{com}_1$ , for  $\text{com}_2$ , and the two combined.

eg Temperature

$T_1$  vary +  $T_2$  low

$T_1$  vary +  $T_2$  mid

$T_1$  vary +  $T_2$  high

Modified 'LTE model - 2comp.py' to output three data sets, the two separate components + combined.

Initial:

$T_1 = 50 \text{ K}$  ;  $T_2 = 50 ; 100 ; 200 ; 300 \text{ K}$

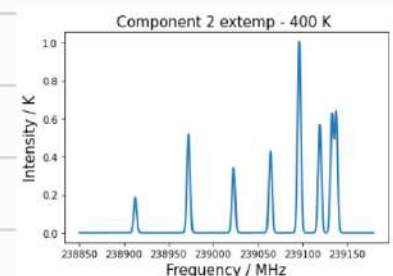
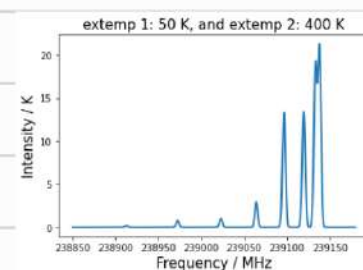
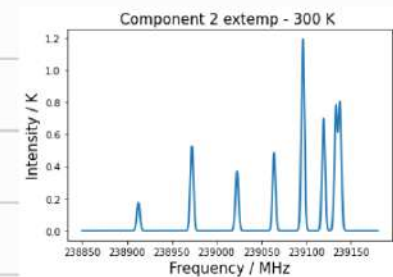
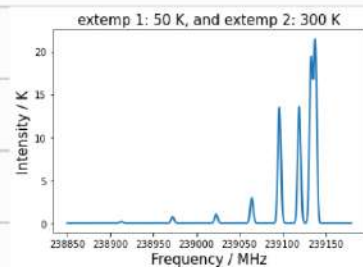
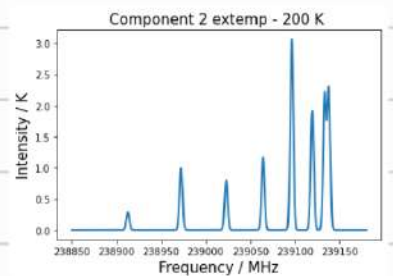
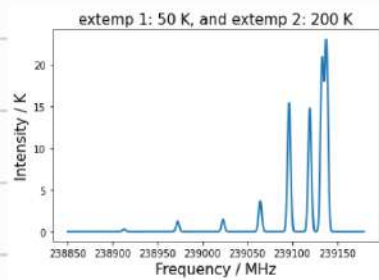
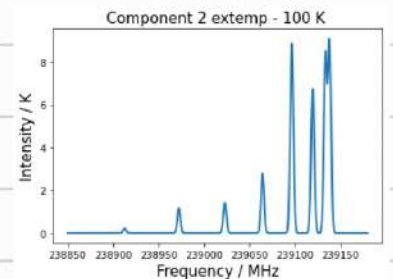
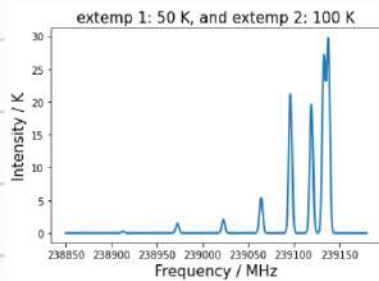
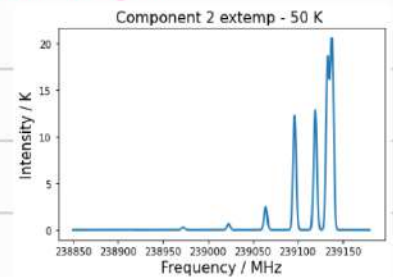
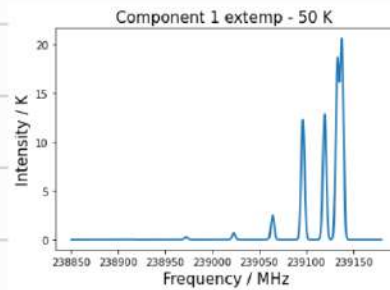
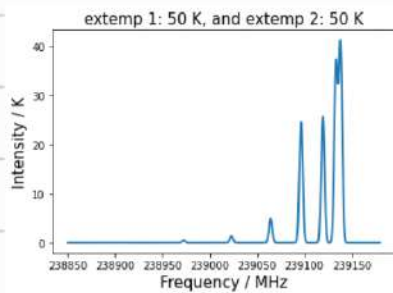
then

$T_1 = 300 \text{ K}$  ;  $T_2 = 50 ; 100 ; 200 ; 300 \text{ K}$

→ don't need to have  $T_1$  at a 'mid' value because  $T_2$  will have a mid value whilst  $T_1$  has some variation.

$T_1 = 50\text{K}$ ;  $T_2 = 80 \rightarrow 400\text{K}$

(note, cannot fit 400K in CASSI)



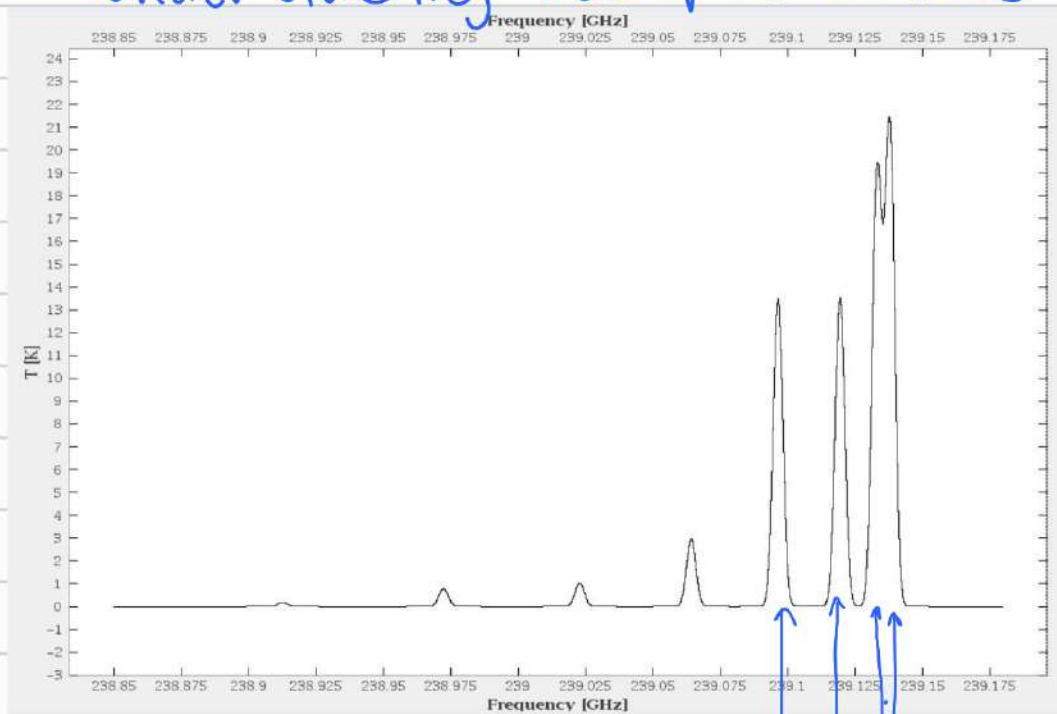


$T_1$  dominates the 'shape'; as  $T_2$  increases, the intensity decreases and so it has little effect on the shape. Though some of the peaks to the left appear (that wouldn't at purely 50K)

The intensity of the combined spectra decreases as  $T_2$  gets hotter, and stops decreasing when it matches the intensity of  $T_1$

20/10/22

Understanding the spectral lines



example  
spectrum for  
demonstration

$J+1 \rightarrow J$   
 $\Rightarrow J_{13-12}$

Remijan 2004

$\text{CH}_3\text{CN}$  is a symmetric top, and its rotational levels are labelled by:

$J$ , the total angular momentum quantum number;  
and

$K$ , the quantum number for the projection of angular momentum along the symmetry axis.

(Note: the vibrational modes are labelled with  $\nu_i$  ( $i = 1 \rightarrow 8$ ). Changes in rotational levels are much smaller than changes in the vibrational states.

In symmetric top molecules, the transitions are classified as parallel when the dipole moment change is parallel to the principle axis of rotation, and perpendicular when the change is perpendicular to that axis.

'Rotational-vibrational spectroscopy'

Issue with CASSIS fitting:

keep finding an inconsistency between the python generated spectra and that of CASSIS.

CASSIS spectra always had a larger intensity, sometimes almost double.

Presumably issue within py code (because CASSIS has huge team).

↳ Might be related to the dilution factor? But both the code and CASSIS calculate it in the same way.



## Meeting with supervisor

To save a spectra (in such a way that we save individual datapoints):

- File
- Save
- Save as file type 'Full Spectrum' (\*.fus)

This saves all generated spectra (ie 'LTE+RADEX') from top to bottom on the RHS of CASSIS in the 'Info Panel'.

Deciding not to debug py code, will just generate spectra in CASSIS.

**\* IMPORTANT \***

for the  $\text{CH}_3\text{CN}$  molecule, CASSIS cannot have a greater Tex. set than 300K.

25/10/22



partial solar  
eclipse @ 1100  
today!

Using CASSIS to generate spectra:

for one or more components, just add the appropriate amount of components and set the desired parameters.

Some default settings:

Range = 238.85  $\rightarrow$  239.175 GHz

Telescope = alma\_400m

$E_{\text{upper, max}} \approx 1000 \text{ K}$

NOT interacting (modelling the two components as 'unmixed' distinct sections of gas)

Continuing two component investigation

essentially repeat the python code steps but now entirely within CASSIS

Initial:

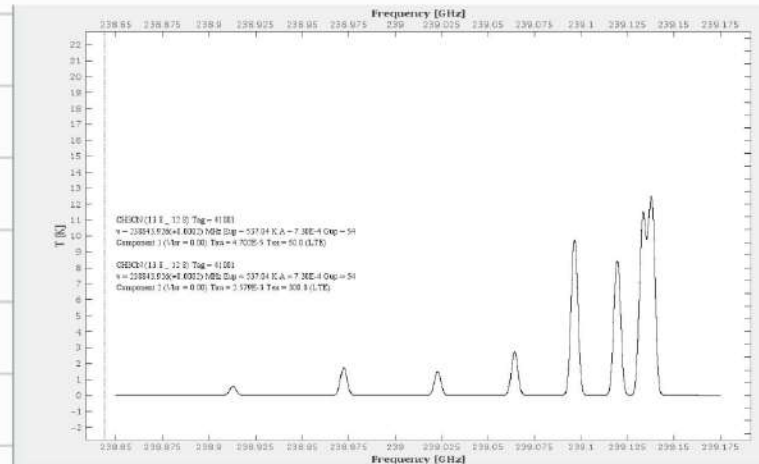
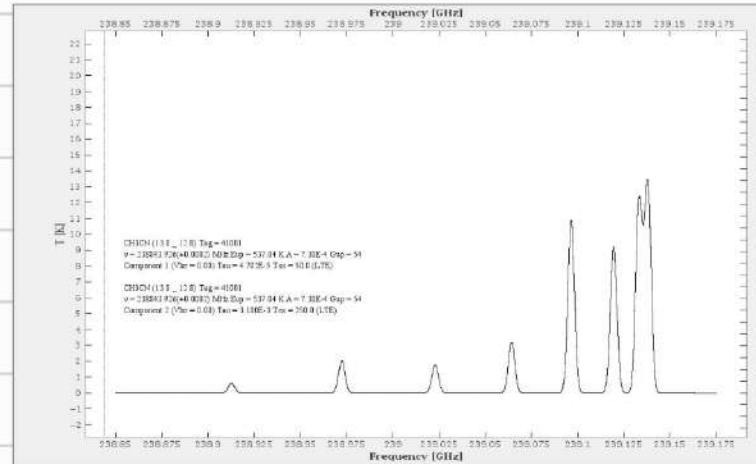
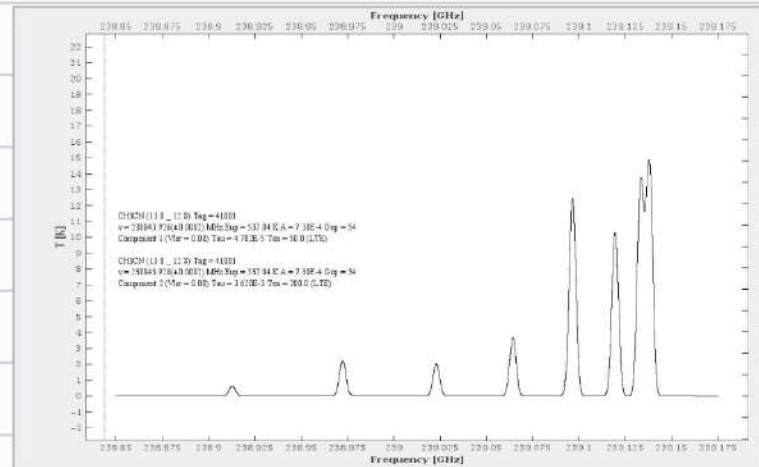
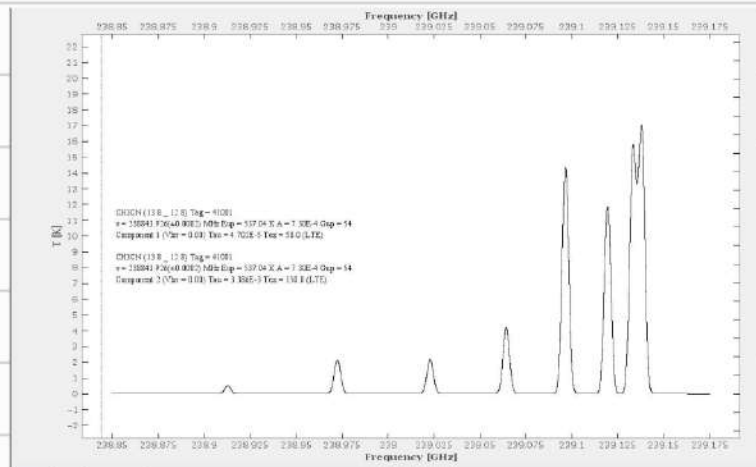
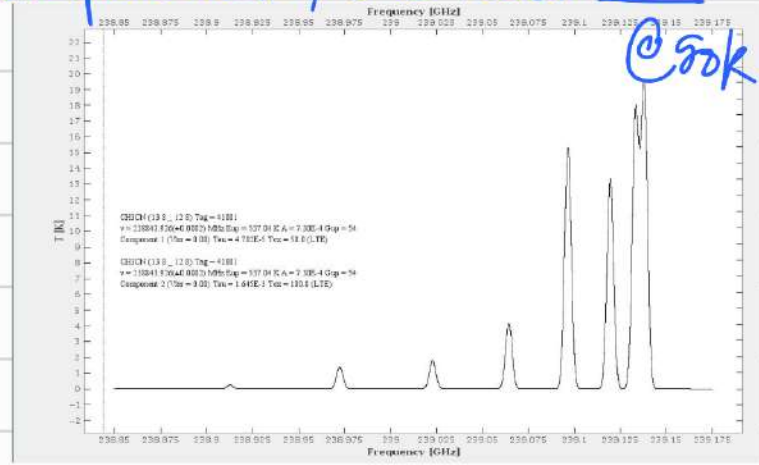
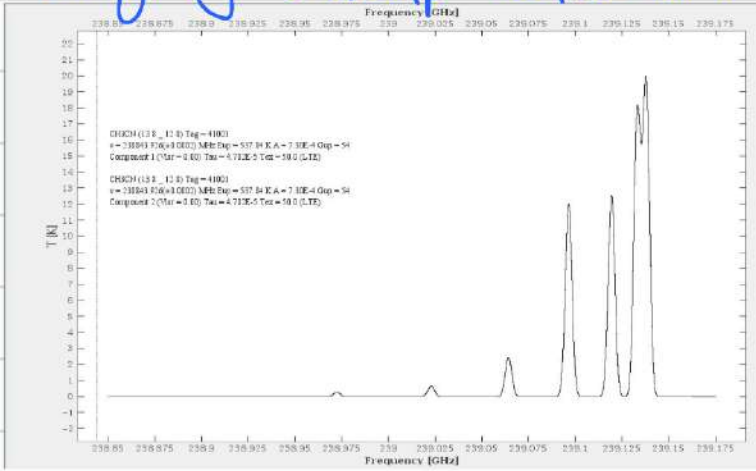
$T_1 = 50 \text{ K}$  ;  $T_2 = 50, 100, 200, 300 \text{ K}$

then

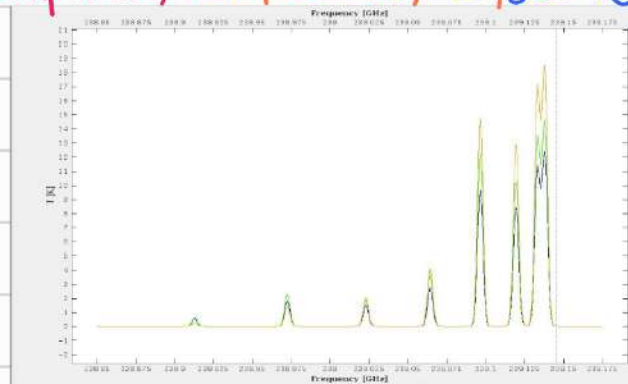
$T_1 = 300 \text{ K}$  ;  $T_2 = 50, 100, 200, 300 \text{ K}$



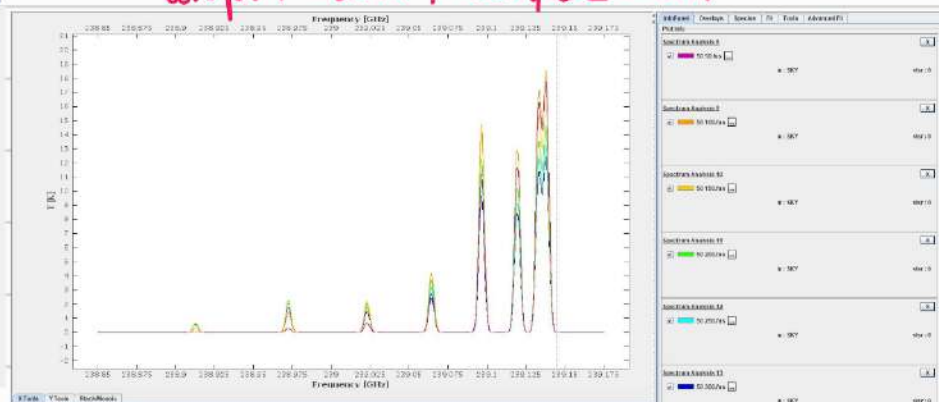
Varying 'extemp' with two components, one held low



Comp.1=50K, Comp.2 = 100, 200, 300 K



Comp.1 = 50K, Comp.2 = all







[illegible]