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

Supervisor : Gary Fuller (g.fuller@manchester.ac.uk)
(gary.a.fuller@manchester.ac.uk)

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

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

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

but $\frac{CH_3CN}{CH_3\,^{13}CN} \neq 50$

Workspace => across bridge in JBCA or ALMA room

NASA ADS

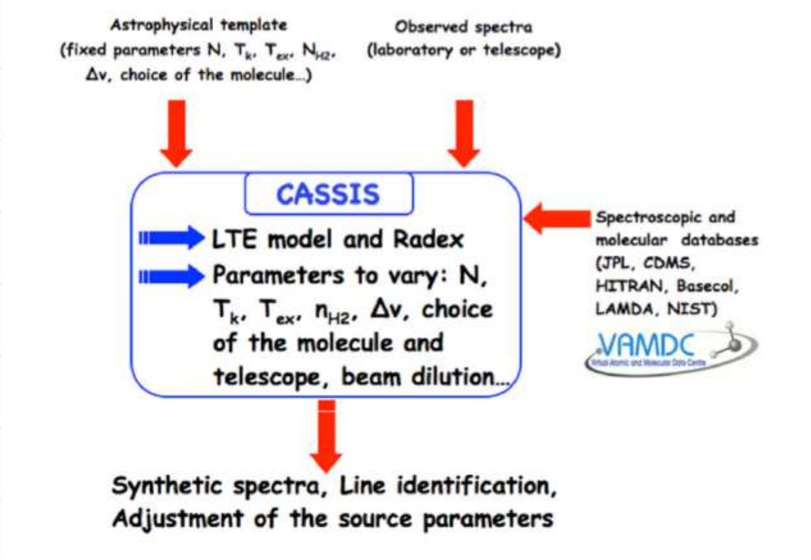
Zoom meeting Thursday?

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
~ 0.67"

Range of sourcelines
Need source-size larger than the beam
can be 0.5 or 2x size

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

Line width does matter

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

LTE - local thermodynamic equilibrium

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/mphys 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 $^{13}C/^{12}C$ at different places in the universe.

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

Section 3

Pg. 13 Single temperature excitation

Column density:

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

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.;
ν = transition frequency;
μ = permanent dipole moment;
S = intrinsic line strength;
$\int T_{mb}\, dV$ = measured integrated main beam density [K·km s⁻¹]

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

☆ Column density $N > 10^6$ cm^{-1}
☆ T > 100 K (but < 500 K (Encyclopedia of Astrobiology, Charley S., 2011)
☆ size: d < 0.1 pc

06/10/22

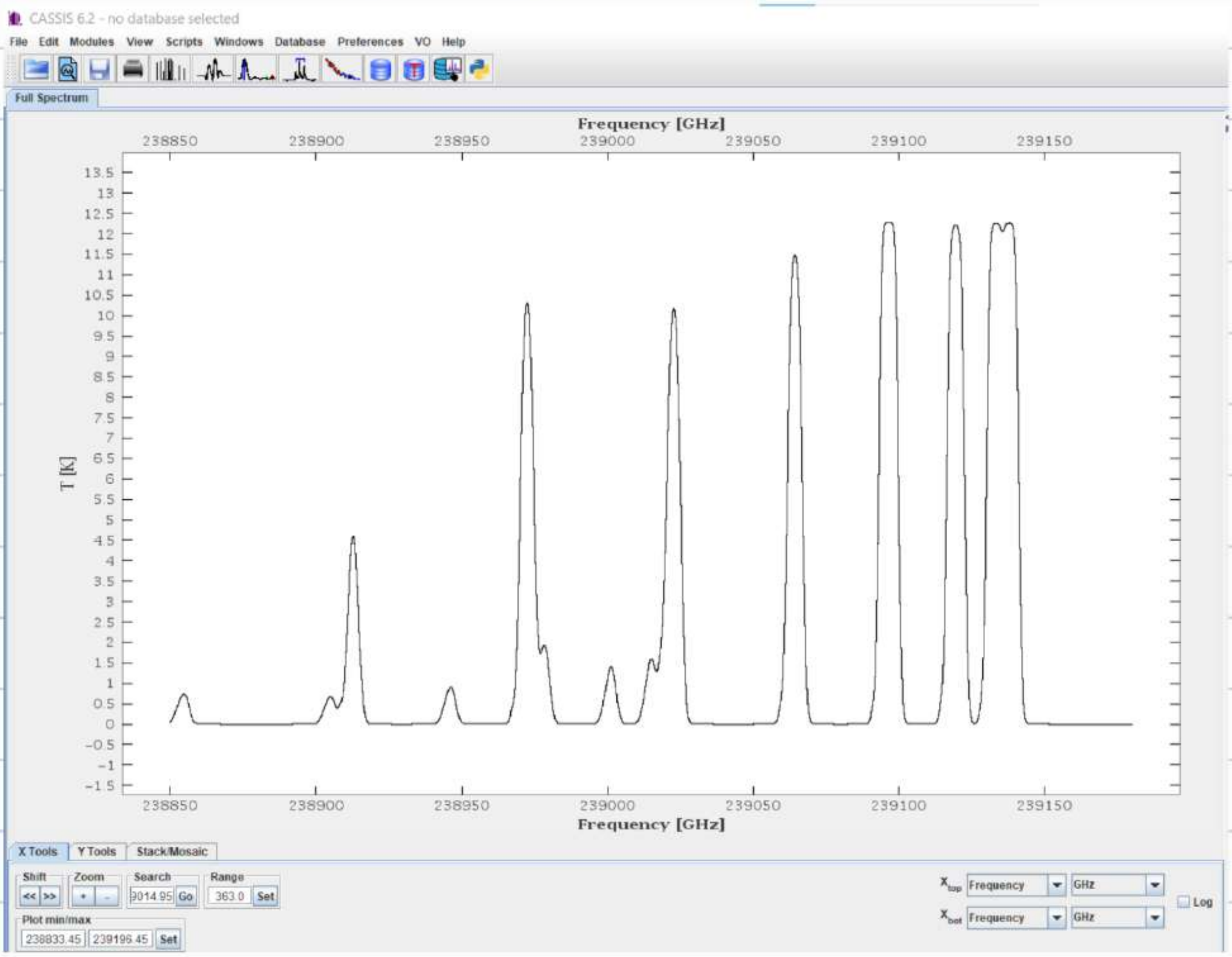
Ran Python 'LTE-model' code to produce simulated emission line spectra of CH_3CN

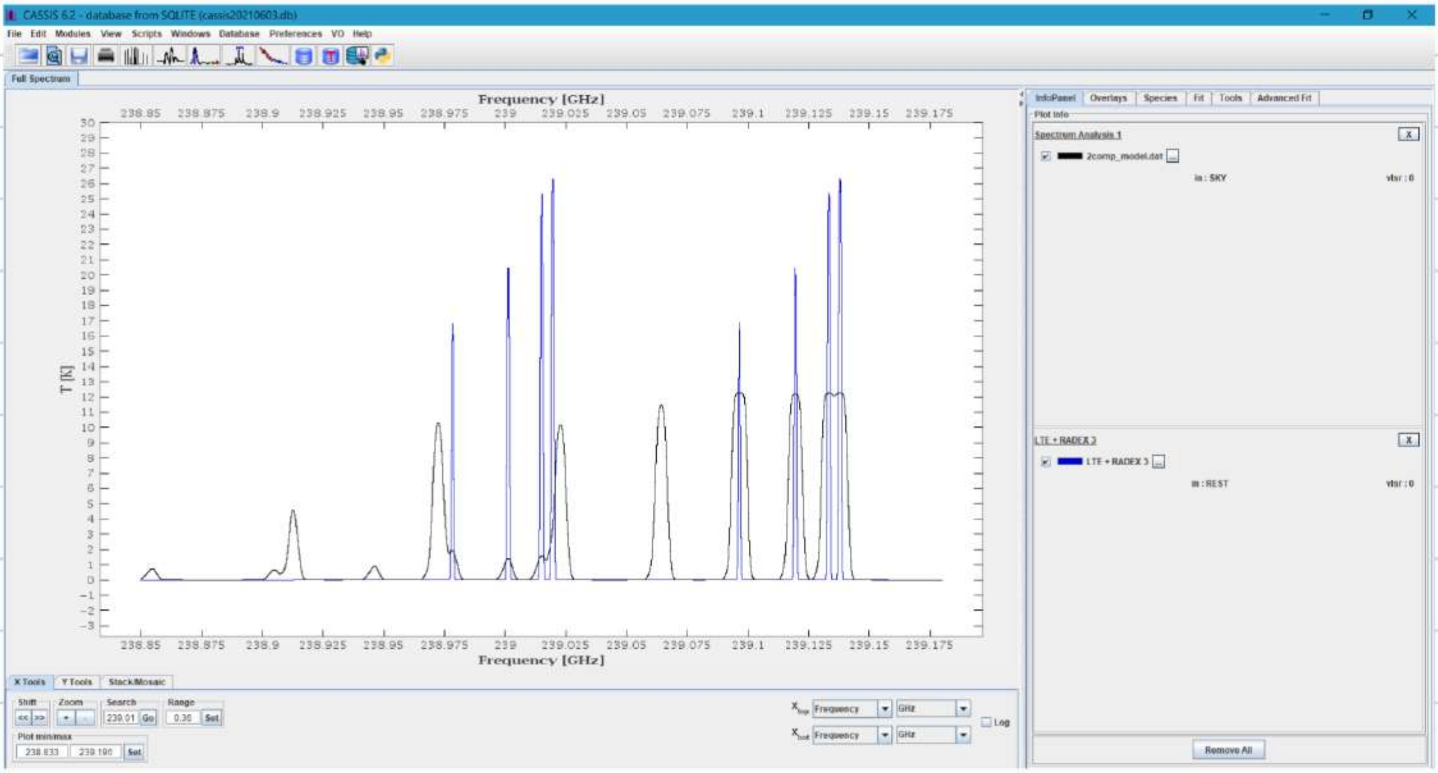
Within code, two molecules (isotopologues of each other) with isoratio of 60.

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

CH_3CN has vibrational states $\nu_1 \longrightarrow \nu_8$
(where ν_1 is the first excited state etc.)

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

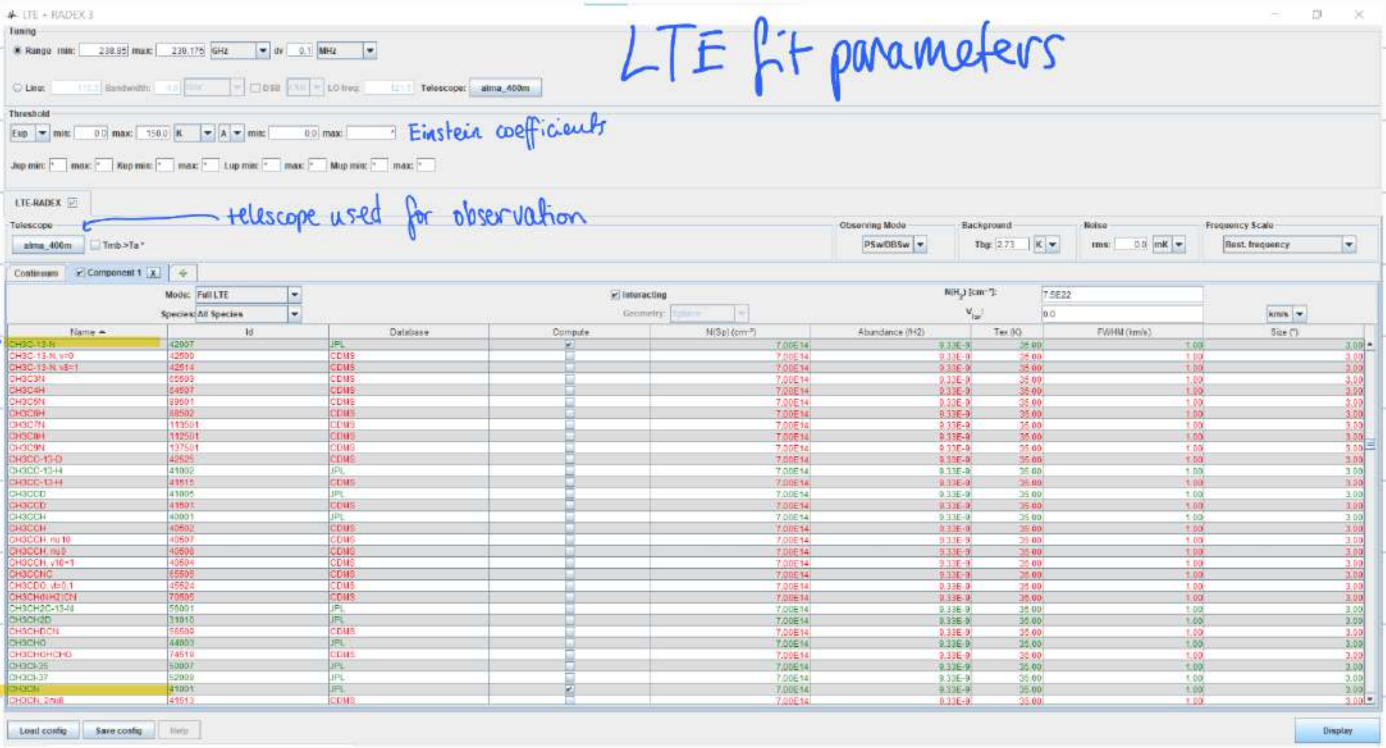




LTE fit parameters

Einstein coefficients

telescope used for observation



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

11/10

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.
ie $T_K = T_B = T_{ex}$

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

flux = specific intensity × solid angle

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

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

col den : $10^{14} \rightarrow 10^{17}$
exc. temp : 20, 30K → 300, 400K
fwhm : 2 → 10
source size : 0.2 → 1. ~ arcsec

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

Gary 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 \ dat files

then eg. \extemp

Variables held constant at

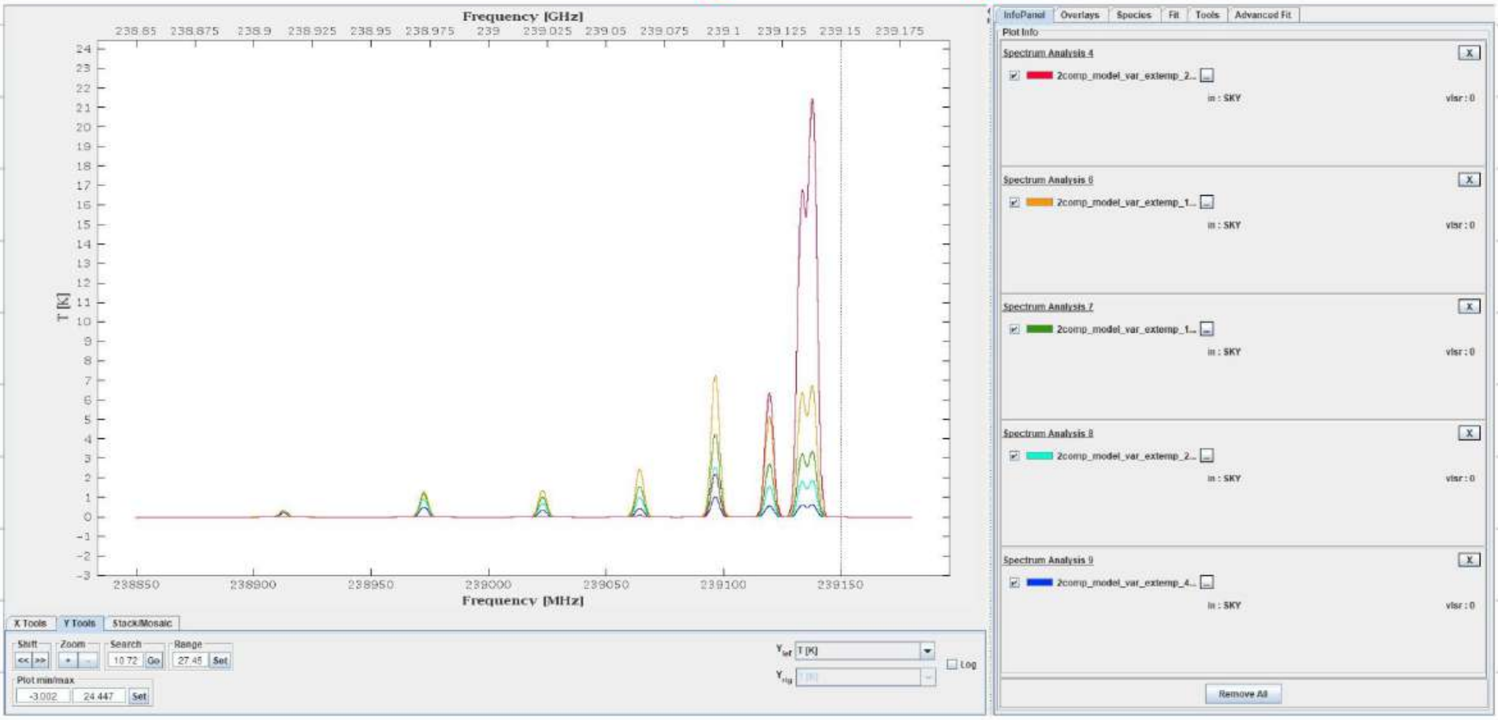
colden = 1e15
extemp = 200
fullwidth = 5
lsr_vel = 0
sourcesize = 0.7
180 ratio = 60

Following changes observed in both CH_3CN and $CH_3{}^{13}CN$:

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. → decreasing intensity



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

$\lambda = \frac{c}{f}$

ALMA (400m baseline)
beam size

(assuming $f = 2.39 \times 10^{11}$ GHz)

$\Rightarrow \lambda = 1.25 \times 10^{-3}$ m

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

$= 0.789''$

13/10/22

Varying two parameters:

So far, our data sets 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

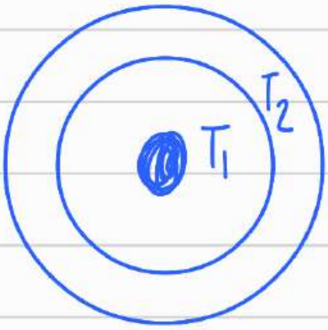
discussions of our findings

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 col·den. 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 rest held constant)



eg
$T_2 < T_1$
$\theta_{T_2} > \theta_{T_1}$

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, Com_1 will be varied for three different values of Com_2.
The combined spectra of the two components will then be analysed in CASSIS by making two separate fits - one with com_1 and another with com_2.
Three spectra will be collected - for com_1, for 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 'LTEmodel-2comp.py' to output three datasets, the two separate components + combined.

Initial:

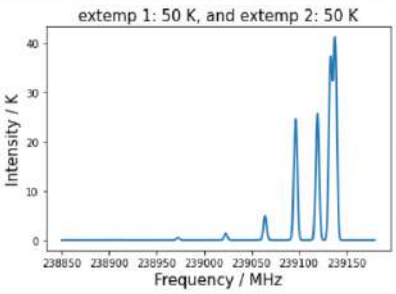
$T_1 = 50\,K$; $T_2 = 50; 100; 200; 300K$

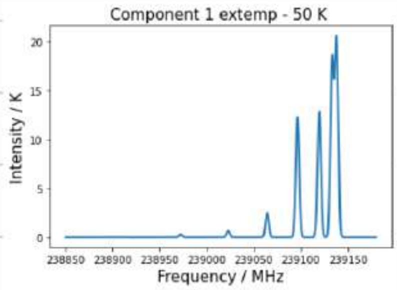
then

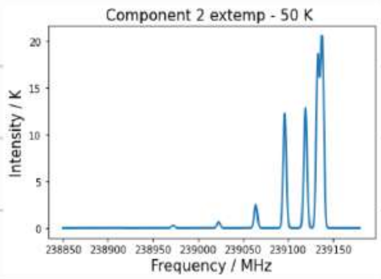
$T_1 = 300\,K$; $T_2 = 50; 100; 200; 300K$

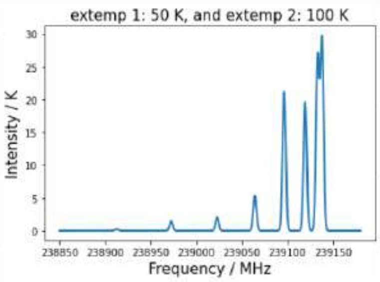
↳ don't need to have T_1 at a 'mid' value because T_2 will have a mid value whilst T_1 has some variation.

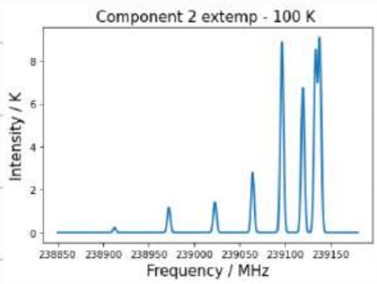
$T_1 = 50K$; $T_2 = 80 \rightarrow 400K$

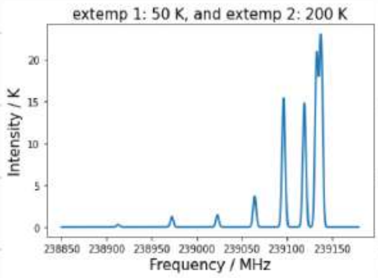


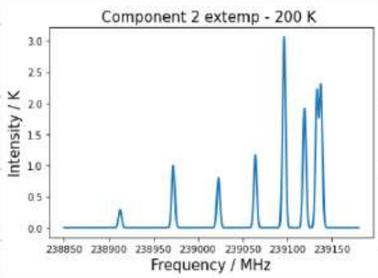


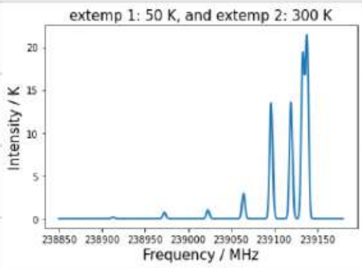


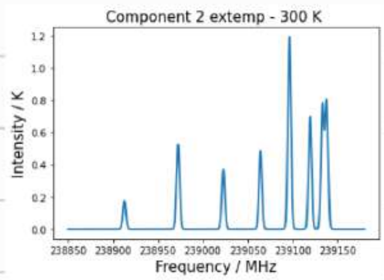


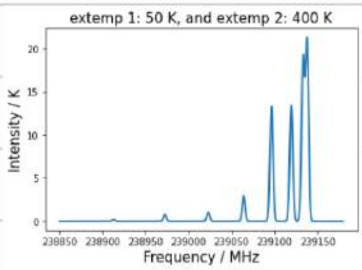


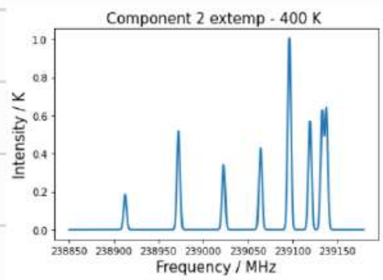










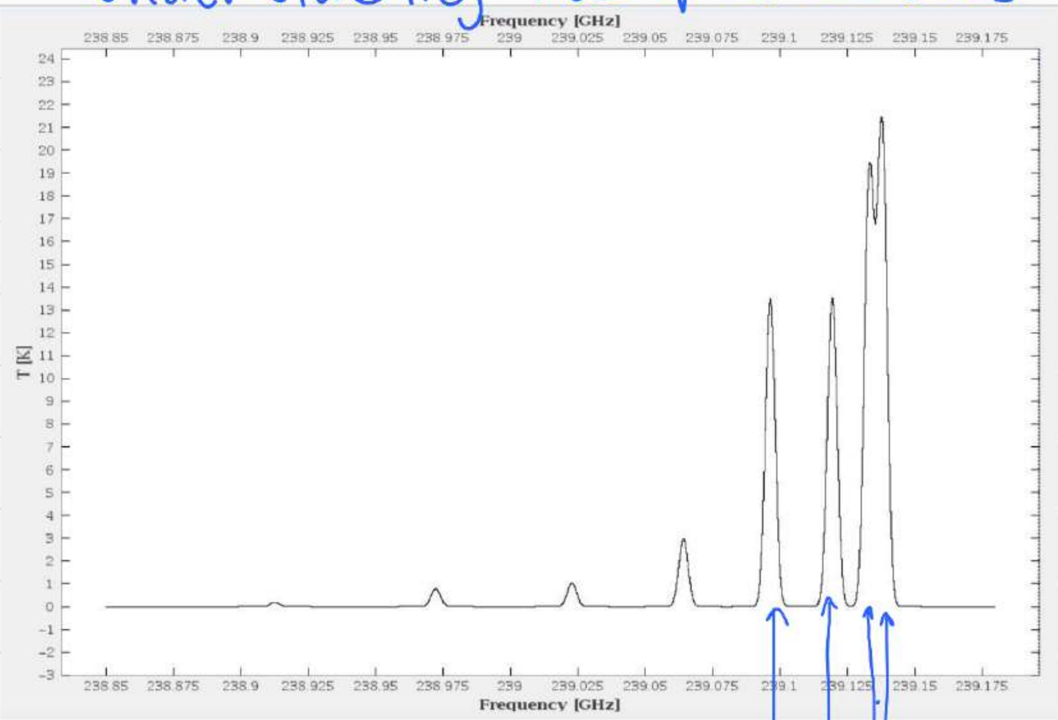


T_1 dominates the 'shape'; as T_2 increases, the intensity decreases and so it has little effect on the shape. Though some of the peaks to the left appear (that wouldn't of purely 50K)

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 spectra for demonstration

K=3

K=2

K=1

K=0

$J+1 \rightarrow J$

$\Rightarrow J_{13-12}$

Remijan 2004

CH_3CN 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 ν_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 'InfoPanel'.

Deciding <u>not</u> to debug .py code, will just generate spectra in CASSIS.