

CASSIS USER MANUAL

CASSIS VERSION 1.1

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USER MANUAL VERSION 1 - 30/12/2006

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Instructions are also available for the more limited version 1.0 of CASSIS.

The instructions for CASSIS 1.1 are gradually being updated. Please check the web newer versions.

The comet model instructions are adapted from J. Crovisier 01/09/2005.

What's new in CASSIS 1.1

A limited LVG model is provided.

The LTE emission and absorption models are merged with the LVG demo to create one single model.

1. Starting remarks

Please note that the 1.1 version of CASSIS has just been released and may have some *teething problems*. The instructions are currently being updated to take into account the changes. We are counting on your feedback to improve future versions both of the program and of the user instructions. We have done our best to eliminate all obvious bugs but since new features have been added recently please send us feedback on any problems that you find with as detailed as information as possible as to what caused them.

The first time you use CASSIS you might find it a little slow as some of the operations involve the transfer of a lot of data. Once the initial setup phase is over it should go faster. More work is required in future to optimise running speed.

These user instructions correspond to the standalone version. The web-based version is not currently working but may be available as a demo later.

Installation instructions for linux and Mac OSX based systems are given on the web with the downloads. It is also possible to install CASSIS on a PC using windows (contact AW or AK, instructions may be available later but producing instruction for PC installation is complicated by differing versions of windows).

We would appreciate greatly that you make reference to CASSIS software when it is used for scientific analysis in published articles or for conference presentations. This will help to support future developments and improvements. Since no published article is yet available about CASSIS software please make reference to our website. If you could also acknowledge the providers of databases and models interfaced to CASSIS this would help to maintain their support and encourage new additions. Full details can be obtained on the web page. Here is a sample text:

"CASSIS software has been used for the analysis. Details can be obtained at http://www.cesr.fr/~walters/web_cassis/references. We have used the following databases xxxx, xxxx and models : yyyyy, yyyyy."

You could also include significant authors, for example:

"We have used the comet model by J. Crovisier."

2. Getting started

You need to have JAVA installed, preferentially Version 1.5. To download java, go to www.java.com

You will also need to install MYSQL (see instructions on website).

For *linux* users: to avoid having to type multiple commands you can create command files for the server and the applet and then run them (e.g. type `./k6s` once the file `k6s` containing the instructions to start the server is created).

Note that CASSIS needs two programmes running simultaneously, the **server and the client (applet)**. You should open the server and the applet from different terminals (first the former then the latter). Information will be displayed in the terminal screens. (Note that a *warn* message does not imply that CASSIS will not continue working.)

Before you start working you need to add a model (click on <add model> and hold down while selecting the model you want).

Note that a turning blue ball indicates that the program is tied up in calculations.

To close a model click on the x in the tab. Be careful not to click on the x when selecting a window to display in the tab bar or the window will close.

3. Operating modes

There are two main CASSIS operating modes:

- 1) *Line-analysis* (Single species line-by-line analysis).

If your spectrum is large this is in general how you will start. You select the chemical species (molecule) you want to analyse. CASSIS will look for all lines of this species one by one in the observations. Results are displayed in the <line spectrum> window. **For details of the *single species line-by-line* mode you should go directly to section 7 of this documentation**

- 2) *Prediction / Global spectral analysis.*

You can use this for predicting spectra. You can also use it for the analysis of spectral scans once you have determined the parameters for each species using the *single species line-by-line* mode. Hence you can check blended lines and search for new species.

Results are displayed in the <full spectrum> window. The global spectral analysis mode may be slow if the spectral scan region is large

4. The full spectrum window

This window shows the results of several models for global analysis (file, LTE/LVG, comets). Note that it is possible to display several models simultaneously. You can select (or deselect) the models displayed by ticking (or unticking) the appropriate box in the *plot_info* pane.

If the whole spectral region is not displayed you can "unzoom" by reverse clicking. (i.e clicking first with the left mouse button then holding down the button and letting it go above left of the first-click position).

You can limit the frequency region displayed by entering the required frequency range and then clicking on the <Set Range> button.

Note that as the number of points that can be displayed is limited (to around 1000) you should be careful to select a frequency range that does not exceed significantly this number of points (i.e avoid tens of thousands of points or more). If you do you will slow down CASSIS unnecessarily. Although not really a bug later versions of CASSIS will be made to warn the user of this problem or to degrade resolution when necessary. This is not presently the case and you should be prudent in the choice of the frequency range you display for the first time.

You can make possible a selection of all files by selecting the option <all files> in the window. You can navigate in the directories in the usual way. When you have located the file you want to download double click it or click open.

The file name should appear next to the <select file> button but nothing will be displayed yet.

You can choose to display the signal or image band.

You can also restrict the frequency range that you want to see plotted by selecting the range in the threshold pane.

Now click on <display selected file>.

Note that if the file is long data processing may take a little time, especially the first time you open it.

You can save the configuration of the file name and path and the selected frequency and read it back later to save time.

Data format:

Observational data can include a multitude of different scans with different backends, resolution, telescopes and gaps in frequency, which can be read and displayed simultaneously. We have tested successfully for the files we have and would appreciate feedback on any problems you encounter.

At present the file must have one of the two following formats (more choice will be provided later – please send us your priorities):

- **CLASS format**

The format supported is that corresponding to versions of CLASS dating from after September 2005. If you have problems reading an older CLASS file first read it with a new version of CLASS and then rewrite it with the new format. If the format of CLASS is changed without our knowledge then CASSIS may not read it – thanks for any feedback.

- **Text format**

See annex 1.

5.2. To display a file:

Once loaded the file should appear in the <full spectrum> window. You can subsequently access this window by clicking on the <full spectrum> tab.

6. LTE emission / LTE absorption / LVG model (LTE+LVG(demo))

A *local thermal equilibrium* and/or *large velocity gradient* model are used to produce a simulated spectrum for predictive purposes. They can also be used to compare observations with a simulation once some idea of the physical parameters of the source is known. For the first analysis of a large spectra containing many species it will probably be easier to work molecule by molecule using the **line analysis** model explained below before comparing the spectrum globally using this model.

At present the LVG model only treats linear molecules.

For details of the LVG model: <http://www.submm.caltech.edu/~vastel/CASSIS/LVG.pdf>

Tuning pane

If you want to work on a single line (or narrow bandwidth) select line and the centre frequency. In this case you can choose to work in single-side-band (SSB) or double-side-band (DSB) by ticking the box. In the latter case you can select lower-side-band (LSB) or upper-side-band (USB). You should also enter the bandwidth in the telescope pane.

If you want to predict several lines over a frequency band select range then select the frequency range in which you wish to simulate the spectrum. (The DSB options are obviously inactivated in this case).

Telescope pane

Here you can select the spectral resolution ($\delta\nu$) for the predictions. Note that high resolution large bandwidth calculations may take some time (and that in extreme cases it is possible to exceed the memory limit giving rise to an error message).

You must also enter the bandwidth if you have selected the line option above.

By ticking the box <Tmb – Ta conv> you can use an *efficiency template* to convert the predictions from Tmb to Ta. The *efficiency template* is a text file giving the telescope beam efficiency at various frequencies. The predictions are multiplied by the efficiency (between 0 and 1) of the closest frequency in the table. The *efficiency template* is part of the *telescope template*. You can select a template for different telescopes in the dragdown menu. It is possible to make your own file.

The *telescope template* also contains the telescope size for the beam dilution calculation (see below). Hence even if you don't use the intensity conversion (to Ta) you should select when possible the correct telescope in the dragdown menu.

You can find out more about **telescope templates** in 8.2.

Threshold pane

Here you can select an energy range for the upper state of transitions to be calculated (for convenience given as an equivalent temperature $T=E/k$). This is particularly important when the molecule considered has a large number of transitions in the frequency region considered. If there are too many transitions to be calculated it may take an excessive time to see the results or in extreme cases the program may stall.

The A_{ij} box also allows the number of transitions calculated to be reduced. The program looks for the line with the highest value of the Einstein constant A. If you enter (for example) 0.1 in the A_{ij} box then lines weaker than 0.1 times the maximum A value will be ignored. This box can be used to work only on the strongest lines or to limit the number of lines when there are a large number in the region considered.

Notes:

- 1) If you display several species simultaneously then the cut-off is calculated for each species separately. For example suppose you enter 0.1. For a species with a maximum A value of $1.5 \cdot 10^{-2}$ the cut-off will be at $1.5 \cdot 10^{-3}$, for another species with a maximum A value of $5.0 \cdot 10^{-4}$ the cut-off will be at $5.0 \cdot 10^{-5}$ and so on.
- 2) The final intensity depends not only on A but also on the upper-state energy and the temperature so that you should not limit A too severely if you want to be sure to see all lines that are strong enough to be observed.
- 3) In both cases (energy and A-value) all lines outside the cut-off value will not appear in the predictions. Hence if there are two lines with similar intensities one just inside the cut-off and the other just outside, only one will be plotted. This can hence lead to a false impression of the spectrum. For example it could give the impression that the spectrum stops dead at some point whereas this is not the case. You should therefore choose the cut-off values with great care if you want to make reliable predictive diagrams.

You can also define a minimum intensity cut-off (in mK) for the lines to be displayed; this avoids plotting weak lines but is not as efficient in reducing processing time since the transition intensity must be calculated before the line is rejected.

Continuum pane

The pane contains a drag down menu where you can select an *absorption template*. This gives the intensity of the illuminating radiation (in K equivalent) as a function of frequency.

The two templates given with CASSIS are only given as an example for testing. Continuum fixes 1K at every frequency point.

Model pane

If you have selected an absorption source below you have the possibility to select or deselect an emission source by ticking or unticking the box. If no absorption source is selected then you must of course have an emission source and you cannot untick the box.

You have three choices for calculating the spectra:

Full LTE: Only an LTE calculation will be made

LTE + LVG: An LVG calculation will be made if possible. If an LVG calculation is not yet available for the molecule selected an LTE calculation will be made.

Full LVG: Only an LVG calculation will be made. If an LVG calculation is not yet available for the molecule selected no spectrum will be displayed for this molecule.

For the molecules for which an LVG calculation is available see: <http://www.submm.caltech.edu/~vastel/CASSIS/LVG.pdf> table 3.

If no *source-template* is selected the *database pane* at the bottom of the screen will be empty.

You can select a *source-template* in the dragdown list. For further details on these templates see section 8.

If load is selected the new-template replaces the last one. If add is selected the new template adds to the last one.

If you select <full database> in the <template> pull-down menu you will see all molecules presently available in the source pane.

You can also <save template> to come back later to a list of molecules and parameters you have already entered.

The LTE model does not depend on the column density of hydrogen. You have the possibility to enter the column density of hydrogen a value so that you can work with relative abundance instead of absolute column density if you prefer. The LTE model only depends on the absolute column density.

Parameters for the LVG model: Number density of hydrogen, ortho para ratio for hydrogen; Presently this parameter only matters for the CO molecule where collisional rate coefficients exist for both spin states. Fraction of helium. Collision with He are taken into account when the helium abundance is given. (See: <http://www.submm.caltech.edu/~vastel/CASSIS/LVG.pdf>)

table 2). By default, the Helium abundance is taken to the interstellar medium value (He/H=0.2).

You can also enter the vlsr (Velocity in the Standard of Rest in km/s) of the source.

Database pane

The database pane shows a list of species (molecules) with an indication of the database containing the linelists. Note that some species may be found in more than one database. You can then choose or use our recommended list (see templates section 8). The tag attributed by the database is also given.

Select the order in which the species are given by clicking on the species, tag, database and collision column headers.

Select one or more molecules for prediction by ticking in the box <comp>. You can remove a molecule from the list by relicking on the tick-box.

You can select/deselect all the species by clicking on the compute column header.

You can also enter the parameters for the predictions.

Parameters for the LTE model are:

*relative abundance**

excitation temperature (K)

velocity linewidth (FWHM km/s) –presently all lineshapes are Gaussian – if you set to zero you will get a line spectrum

source dimension (in arc seconds for beam dilution calculation)

*column density** (cm⁻²)

* either one or the other is automatically calculated according to the entered value for the H₂ column density

and for the LVG calculation

kinetic temperature

Note that in the LVG computation the kinetic temperature must be within the range chosen for the corresponding molecule (see :

<http://www.submm.caltech.edu/~vastel/CASSIS/LVG.pdf> table 2)

Note that the excitation temperature will have no effect on the LVG computation and the excitation temperature will have no effect on the LTE computation.

In the future, CASSIS will be able to introduce a background source (temperature and filling factor) and compute the contamination for the emission of the foreground molecular cloud. Presently we only consider the contribution of the cosmic blackbody radiation, set equal to 2.7 K in all calculations.

New: You can enter parameters for the entire column by clicking on the appropriate column header.

A beam dilution calculation is included in the predictions using the telescope diameter in the *telescope template* and the source diameter for each species. If this correction is not required then the source size should be set to a large value (so that it is larger than that of the telescope beam).

You can find out more about **telescope templates** in 8.2.

Absorption-source pane

This model calculates the absorption spectrum of an object situated in front of a continuum source. As yet only the LTE model is available.

The layout of the window is very similar to that of the emission model.

The pane contains a drag down menu where you can select an *absorption template*. This gives the intensity of the illuminating radiation (in K equivalent) as a function of frequency.

The two templates given with CASSIS are only given as an example for testing. Continuum fixes 1K at every frequency point.

You can make your own *absorption template*. The spacing of the grid of frequency points is free. CASSIS will linearly interpolate between the two closest points. If you choose a finer grid then calculations will be more precise but slower.

You can find out more about **absorption templates** in 8.3.

Command pane

Once all the parameters are correctly entered click on <display> to see the result of the simulation (and compare it with the observations if you have already entered a file). For details of the display graphics see section 4.2.

You can save the configuration by clicking on save-configuration and giving a file-name. You can reload the configuration by clicking on load-configuration and selecting the appropriate file name.

An example of how the configuration is saved is given in annex 2.

7. Line analysis

Plotting pane

For this model you must have a file of real data to be compared with the predictions. Click on <select datafile>. Then choose the file from a directory in your computer. The filename will appear next to the <select datafile> button.

You can choose to display lines sorted in order of:

- increasing frequency
- increasing upper-state energy (E_{up})
- decreasing A_{ij} (Einstein coefficient).
- decreasing intensity

by choosing the appropriate option in the dragdown menu.

You can choose the signal or image band.

Threshold pane

The comparison with the predictions is limited to the frequency interval of the observations in the file you have entered. You can further reduce the frequency limits in which you want to work by entering the minimum and maximum frequency.

You can enter the cut-off energy of the upper state for the transitions to be calculated (for convenience given as an equivalent temperature $T=E/k$). This is particularly important when the molecule considered has a large number of transitions in the frequency region considered. If there are too many transitions to be calculated it may take an excessive time to see the results or in extreme cases the program may stall.

You may also want to enter a minimum energy for the transitions to be calculated.

You can enter the bandwidth to be displayed around each line.

The A_{ij} box also allows the number of transitions calculated to be reduced. The program looks for the line with the highest value of the Einstein constant A . If you enter (for example) 0.1 in the A_{ij} box then lines weaker than 0.1 times the maximum A value will be ignored. This box can be used

to work only on the strongest lines or to limit the number of lines when there are a large number in the region considered. Note that the final intensity depends not only on A but also on the upper-state energy and the temperature so that you should not limit A too severely if you want to be sure to see all lines that are strong enough to be observed.

Species pane

If you have selected <full database> in the <template> pull-down menu you will see all molecules presently available.

For further details on the templates see section 7.

To choose the molecule you want to model you click on the row in the table corresponding to this molecule so that it becomes yellow.

Model pane

By ticking the box <Tmb – Ta conv> you can use an *efficiency template* to convert the predictions from Tmb to Ta. The *efficiency template* is a text file giving the telescope beam efficiency at various frequencies. The predictions are multiplied by the efficiency (between 0 and 1) of the closest frequency in the table. The *efficiency template* is part of the *telescope template*. You can select a template for different telescopes in the dragdown menu. It is possible to make your own *telescope template* file. You can find out more about **telescope templates** in **10.2**.

A beam dilution calculation is also included in the predictions. The beam width of the telescope is taken from the telescope template in the dragdown window. You need to enter the correct source diameter (in arcseconds – see below). If this correction is not required then the source size should be set to a large value (so that it is larger than that of the telescope beam).

The oversampling box concerns the number of points in the prediction. For example an oversampling of 3 (default) means that there are three times as many points in the prediction as in the observation file. If the oversampling is too small the resolution will be reduced the prediction will not be smooth and in extreme cases lines will not be seen. If the oversampling is too large then calculation times will be long and in extreme cases the program may stall.

Emission source pane

The model allows you to add the results of up to three physically different components with different parameters (e.g. hot core and cooler outer region).

By default only one component is selected. Tick in one or two of the other boxes if you want to add more components.

You can then enter your best estimation of parameters for each of the physical components of the source). These parameters are absolute column density (cm^{-2}), kinetic temperature, linewidth (FWHM in km s^{-1} , presently lines are supposed Gaussian.), source size in seconds.

The first component in the list takes the vlsr from the observations file. For the other two components you can choose the vlsr (in km/s) separately.

Other species pane

By ticking on the other molecules box you will also see the position of the lines of other species which are in the plotted frequency interval around the species of interest. Note that only the position is given and no indication of intensity is included in this version of CASSIS. However you can limit the intensity of lines indicated with the $A_{ij} > A_{ijmax}$ box and by choosing a cut-off energy (see above).

Note that the cut-off is calculated for each species separately. For example suppose you enter 0.1. For a species with a maximum A value of $1.5 \cdot 10^{-2}$ the cut-off will be at $1.5 \cdot 10^{-3}$, for another species with a maximum A value of $5.0 \cdot 10^{-4}$ the cut-off will be at $5.0 \cdot 10^{-5}$ and so on.

You can also limit the lines plotted by making your own *other_species_template* containing only those species you feel are important in the object you are looking at. Choose the template to be used in the dragdown menu. If you don't have a specific template its advisable to use the ISMLattWalt template which avoids predicting the same species from both CDMS and JPL databases.

Display pane

Click on display model to see the results. The first line in the series will appear.

You can save the configuration by clicking on save-configuration and giving a file-name.

You can reload the configuration by clicking on load-configuration and selecting the appropriate file name.

7.1. The *line spectrum* window

This window shows the observations plotted as a histogram.

It also shows the predictions. If the check-box *lines* is selected the predicted centre frequency will be displayed as a vertical line. If the check-box *Gaussians* is selected the predictions are plotted as a histogram assuming a Gaussian line shape. If the check-box *other species* is ticked the presence of transition of other molecules in the frequency domain plotted will be shown.

In the window you have information on the central transition of the species you are working on: the quantum numbers (in the format used by the databases – read the relevant information given on the database websites), the energy of the upper state of the transition (E/k in K), the Einstein A coefficient and the optical depth (τ) of the line.

You can move from line to line by clicking on the arrow keys at the bottom or by typing in the number in the series of the line you want to see.

You can go back and change the parameters by clicking on the < Line analysis > tab.

7.2. Fitting a Gaussian

Make sure that the *Line fitting* box is selected by clicking on it if necessary. Define the horizontal limits of the line to be fitted using the **right** mouse button (click and hold-move-release). This is shown by a grey-blue area. (Note that on certain computers the indication of the blue-grey box may need a slight delay.)

Once the area is defined the integrated intensity (moment in K/kms^{-1}) is displayed for the part of the observations selected. Note a minor bug in this version the moment will not change when you change lines unless you redefine the area.

Click on <fit Gaussian> to obtain the fit.

The fitted line will then be shown and the result of the fit will give :

The maximum intensity (in K).

The velocity shift of the line (in kms^{-1}).

The line-width (FWHM in kms^{-1})

You can also get these parameters in the applet dialogue box by clicking on <write log>. If you do this for successive lines you will get the results in the form of a table. The table also gives the integrated intensity (flux) for the Gaussian line fitted. You can compare this value with the moment of the observations (see above). At present we leave it to the judgment of the user to decide which if either of the intensity measurements is the most appropriate and what corrections are to be made.

If you want to fix a parameter, enter the fixed value in the corresponding value-box and check box next to it (shown by a tick).

If you think two or more lines are convoluted you can add a second Gaussian by checking the box *Gaussian 2* and additional Gaussians by clicking <add Gaussian> then checking the corresponding box.

8. Templates

8.1 Source Templates

If you have selected <full database> in the <template> pull-down menu you will see all molecules presently available. The data is taken from the CDMS and JPL catalogues with a few corrections in order that it all be in the same format. For some species a separate entry created (by Charlotte VASTEL) treats ortho and para species separately.

Other templates are available. For example you can choose to work only with the JPL or with the CDMS database. Some templates may only be for test purposes. We also provide a template (authors Valerio LATTANZI, Adam WALTERS) with the recommended entry from the databases available for each known or supposed potential ISM species. If this template is not included in your CASSIS package then you can download it at:

http://www.cesr.fr/~walters/web_cassis/templates.htm.

The criteria for our choice and other useful information are given in the table summarising the databases given on the CASSIS website:

(http://www.cesr.fr/~walters/web_cassis/Divers/Molec_tab.pdf).

Please send any feedback on this template to walters@cesr.fr.

You can add several templates by clicking on the <add> button then selecting the template to be added.

You can create your own templates. Templates can only be saved in the ETL model but they can later be used in both the ETL and ETL-line models.

To create a template select the molecules that interest you in the ETL model by clicking the <compute> box. You can also enter your chosen default parameter values for these molecules. Save the template by selecting <save templates> in the template pull down menu then entering a name for the template in the dialogue box. The template should appear in the list.

To delete a template select <delete template> in the template pull down menu, enter the name of the template to be deleted in the dialogue box and confirm the action. Be careful not to delete one of the major templates that you might need later.

We hope that CASSIS users will provide some of their own templates as standard templates for other CASSIS users – credit will be given – please contact a member of the CASSIS team if you would be willing to do this.

Molecules in the table can be arranged in different ways by clicking on the column header. For example by clicking on tag you can arrange them by increasing tag or decreasing tag.

8.2 Telescope templates

These can be found in the subdirectory /web/telescope of the directory where you have saved the CASSIS code after download. Here is an extract of the *Iram* template:

```
// Diameter (m)
30
// Frequency (MHz), Beam efficiency, IF (GHz), LSB gain (%), USB gain (%)
0.0000 0.88118      2.9960 1.0000 1.0000
5000.0 0.87645      2.9960 1.0000 1.0000
.....
95000 0.76924      2.9960 1.0000 1.0000
1.0000e+05 0.76205      2.9960 1.0000 1.0000
1.0500e+05 0.75474      2.9960 1.0000 1.0000
.....
```

The first line is a comment line, reminding you that on line 2 can be found the telescope diameter in m.

Line 3 is also a comment line and gives the column headers for the remaining lines.

(here stands for other similar lines not given in the extract).

The telescope diameter is used for beam dilution calculations. *Intermediate frequency* is used for the double side-band frequency calculations. Other parameters are used for converting T_{mb} to T_a .

You can edit these templates or make your own. The spacing of the grid of frequency points is free. CASSIS will linearly interpolate between the two closest points. If you choose a finer grid then calculations will be more precise but slower.

8.3 Absorption templates

These can be found in the subdirectory /web/continuum of the directory where you have saved the CASSIS code after download. Here are the first few lines of power0303:

```
0.00000 0.00000
10.0000 2.00909
20.0000 2.47863
30.0000 2.80264
40.0000 3.05791
.....
```

The two columns are frequency in GHz and illuminating radiation in K equivalent.

Power0303 given only as an example uses a simple power law.

You can make your own *absorption template*. The spacing of the grid of frequency points is free. CASSIS will linearly interpolate between the two closest points. If you choose a finer grid then calculations will be more precise but slower.

9. Comet model (text not totally updated to 1.0)

The comet model is derived from the *PAPSYNTHE* software developed by the "comet team" at Observatoire de Meudon for the preparation and quick-look analysis of radio spectroscopic observations of comets (see e.g. Crovisier et al., 2004, A&A, 418, 1141).

The test comet spectrum provided by CASSIS is a spectrum of comet C/1995 O1 (Hale-Bopp) observed at the CSO on 21 Feb. 1997, showing lines of CH₃OH, SO and HC₃N (Lis et al., 1999, Earth Moon Planets, 78, 13).

9.1. Getting going

If you have measured data you can load it as explained in 2.

To run the comet model in the <add model> tab and select <comet model>.

9.2. Model assumptions.

Simple LTE excitation with a unique temperature is assumed.

The average molecular column densities are evaluated assuming spherical symmetry with molecules produced from the comet nucleus, radially expanding with a uniform velocity V_e , and destroyed by solar UV with a rate $\beta \cdot R_h^{-2}$. (This is the so-called "Haser model" for parent molecules.)

9.3. The comet model window - Model parameters.

9.3.1. General parameters (top part of the screen)

- min and max frequencies [MHz] of the frequency interval to which the model is applied.

- frequency resolution [MHz] of the synthetic spectrum. Default value is 1 MHz.

- water production rate Q of the comet [molecules s^{-1}] (this parameter controls the global gas production of the comet). Default value is $5.E29$ molecules s^{-1} .
- distance R_h of the comet to the Sun [AU] (this parameter is used to estimate the effective photodissociation rate). Default value is 1 AU.
- distance Δ of the comet to the Earth [AU] (used to estimate the linear field of view and the column densities). Default value is 1 AU.
- expansion velocity V_e [km/s] of the cometary atmosphere (used to estimate the line' widths and the molecular column densities).

9.3.2. Parameters for each molecule.

These parameters should be specified for each molecule selected for the model in the scrolling list at the bottom of the screen.

You have a list of all molecules in the JPL and CDMS databases. By clicking on the headers the list can be arranged by name, tag, molecules selected etc.

Select one or more molecules by ticking in the box <comp>. You can remove all the ticks by clicking on <deselect all>.

- abundance; this is the production rate of the molecule relative to water. Actual production rate of the molecule is $Q \cdot \text{abundance}$.

- temperature. Default value is 77 K.

- the linewidth is twice the expansion velocity

- photodissociation rate β [s^{-1} at $R_h = 1$ AU]. The default values which are provided are taken from Crovisier (1995, J. Geophys. Res., 99, 3777); when this rate is unknown, $\beta = 1.E-4$ s^{-1} is assumed.

Once all the parameters are correctly entered click on <display comet model> to see the result of the simulation (and compare it with the observations if you have already entered a file).

9.4. Model limitations.

This simplistic model is limited to quick-look analysis. More realistic models should be used for more reliable interpretations.

The model, valid for parent molecules released from the nucleus, is not valid for secondary products such as radicals and ions which are photolytic products. The model, however, could still be useful for evaluating relative line intensities of these species.

10. Rotational diagram

Note: the rotational diagram has not yet been fully tested. It should therefore only be used if you have previous experience in this type of analysis. In particular you should take care to enter correct integral intensity values (flux). No corrections are presently made to the flux (e.g. for beam dilution) and you should make these corrections yourself. Please check carefully any results obtained and send feedback if you encounter any problems or have suggestions.

You can launch the rotational diagram either from the CASSIS applet by clicking on <rotational diagram> or independently from a terminal window as explained on the website.

You then need to enter a text file with the following format:

*Name of molecule;Tag
Frequency;Flux;Uncertainty in the flux*

Repeating the last line as many times as you have measurements.

Example (for the format of the file only, numerical values arbitrary):

```
H2CO;30501  
216568.651;0.991;0.1  
218222.192;14.721;0.05  
.....  
.....
```

Note that it is important to enter the correct tag of a molecule in the databases as this is used along with the frequency to find the correct parameters (upper state energy and degeneracy) for the transition causing the line. Also at present you should type the frequency exactly (in general with three decimal places) as it appears in the database entry. You can get these frequencies either from the database itself or from the terminal window for the applet when you are measuring the fluxes.

Assuming that you have corrected the fluxes appropriately, that the transitions aren't optically thick and that the assumption of ETL is valid you should obtain a straight line. A least squares fit to this line gives the excitation (rotational) temperature and the column density for the species as appears in the bottom right box.

If you wish to use a correctly weighted least-squares fit then you should take care to enter realistic values for the flux uncertainties. Only if these uncertainties are realistic will the uncertainty on T and N be given correctly.

In some cases you will want to include only certain points in the least square fit. The procedure is as follows:

1. Draw one (or if necessary) several rectangles around the points you want to include by clicking once at the start and finish position of the rectangle.*
2. When you have finished press <close selection> .
3. Press <display> to see the results of the least-squares fit.

You can start the present series again by clicking <reset this selection>.

If you think you have several regions in your source (example hot core and cooler outer region) which show up independently as a function of energy you can define groups of points as explained above and get parameters for all of them simultaneously.

You can restart the whole analysis by pressing <reset all selections>.

* Note that holding down the mouse-button while moving it will not define the rectangle but lead to a zoom as for other graphics in CASSIS. You can zoom out by reverse clicking (i.e clicking then holding down the left button and letting it go above left).

Annex 1 – Text format for observations

Example:

```
DM_Tau  HDO(101-000)  JCMT-DAS
// comments
// comments
97  46924.5200  456923.2410  0.3125  5.5010
0.069219  464910.0000  456937.7813
-0.076309  464910.3125  456837.4687
.....
.....
DM_Tau  HDO(101-000)  CSO-AOS4GHz
// comments
// comments
140  893638.666  890638.666  0.2189  -4.0
0.069219  464910.0000  456937.7813
```

.....
.....

etc.

The format is as follows:

First four header lines:

Line 1 (used for display purposes): *object_name transition_name instrument_name*

Line 2 (comment line), must start with // *any useful comments and parameters for information*

Line 3 (comment line), must start with // *any useful comments and parameters for information*

Line 4 (parameter line):

number_of_points_in_subset instrument_tuning_frequency(signal)

instrument_tuning_frequency(image) frequency_resolution vlsr(km/s)

Then the data lines:

Tmb (or Ta) in K frequency in MHz(signal) frequency in MHz(image)

..... repeat for the number of frequency points.

Repeat from header lines for each data subset with differing parameters (telescope, vlsr, etc.)

Notes:

transition_name. This assumes you are working on a single transition of a given species, if not you can give other information, e.g "spectral_survey_Orion"

number_of_points_in_subset. The number of lines of data in this subset i.e. before the next header to change parameters (or the whole spectrum if only one subset).

instrument_tuning_frequency(signal). (MHz) this will be used for the calculation of the velocity scale of the signal band. If not available give:

$(\text{maximum signal frequency} - \text{minimum signal frequency})/2$

instrument_tuning_frequency(image). (MHz) this will be used for the calculation of the velocity scale of the image band. If not available give:

$(\text{maximum image frequency} - \text{minimum image frequency})/2$

If you don't know this use the same value as the signal band.

frequency_resolution. Use of subsets with different headers allows the simultaneous plot of sub-scans with different resolution

Tmb (or Ta). In order to best compare with the predictions (which can take into account beam dilution) you need to enter Tmb. However if you only have Ta you can enter this to start the analysis and make the correction later. If you have a complicated source structure you can work iteratively.

frequency in MHz(image). If you don't know this just copy the value for the signal band.

If you observe an error it may be that your file contains additional characters like ^M added by windows and not appearing in certain editors. Although we think that we successfully filter these characters please signal precisely any problems encountered

Annex 2 – example configuration file

```
LTE
frequencyMode 1
rangeMin 115.0
rangeMax 116.0
line 115.271202
dsb 1
dsbMode LSB
telescope jcmt
tmbBox 0
efficiency jcmt
bandwidth 4.0
resolution 0.1
eupMin 0.0
eupMax 150.0
aij 0.1
imin 0.0
density 7.5E22
vlsr 0.0
template Full CDMS
```

Annex 3 – updating databases

YOUR_MYSQL_DIRECTORY: usually /usr/local/mysql on Linux and Mac installation.

YOUR_CASSIS_DIRECTORY: the directory where cassis.zip was unzipped.

You can first load CASSIS database content using our static database archive: database_content.sql.gz (40Mo - 240Mo deflated) that should be included in your CASSIS package or downloadable on the web:

```
cd YOUR_CASSIS_DIRECTORY/sql/
gunzip database_content.sql.gz
YOUR_MYSQL_DIRECTORY/bin/mysql -u cassis cassis < database_content.sql
```

(With some operating systems the file *database_content.sql* may be unzipped during download so that the unzip operation is unnecessary).

Note that the operation may take several hours. The only indication at the beginning that it is running is the non-display of the cursor after typing the command line. The cursor will appear once download is complete

You can also update the databases directly from their websites (you must be connected to internet):

```
cd YOUR_CASSIS_DIRECTORY/server/  
java -Xss1024k -Xms512m -Xmx512m -jar cassis.cassisd.jar -u
```

Database updating is controlled by the contents of *sql_update.properties* which can be found in the */web* folder and changed using a simple text editor. Help is given in this file as comments.

Other help can be obtained by including the `-h` option on the java command line. In this way you can also see some other options for the "advanced user" – (it's best not to use these options if you don't know what you are doing).

You can include an access to your personal databases, which must however be in the same format as that of JPL/CDMS.

```
databaseUpdate[n] = 0 do not update  
                  = 1 force update
```

Note that the update process involves reloading the whole database (if selected with 1) and needs continuous connection to the internet during several hours.

Annex 4 – user instructions version history

1.1-1 first version for CASSIS 1.1

Annex 5 – abbreviations

vlsr – velocity relative to local standard of rest
FWHM – full width half maximum