



# Formalism for the CASSIS software

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## I. Radiative transfer

The intensity of a source emitting in the interstellar medium along a line of sight  $I_\nu$ , will change if the radiation is absorbed or emitted, and this change can be described by the equation of transfer :

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu \quad (1)$$

where  $\frac{dI_\nu}{ds}$  represents the change of the intensity  $I_\nu$  at the corresponding frequency  $\nu$  through a slab of material of thickness  $s$ . It depends on the absorption coefficient  $\alpha_\nu$  and the emissivity  $j_\nu$ .

In Local Thermodynamic Equilibrium (LTE) the intensities of emitted and absorbed radiation are not independent. The Einstein coefficients give a convenient means to describe the interaction of radiation with matter by the emission and absorption of photons.

Consider a gas containing atoms with discrete energy levels  $E_u$  and  $E_l$ . According to Einstein (1916), a system in the excited state  $E_u$  will return spontaneously to the lower level  $E_l$  with a certain probability  $A_{ul}$  such that  $n_u A_{ul}$  is the number of such spontaneous transitions per second in a unit volume, with  $n_u$  the density of state  $u$ . The difference in energy between transition  $u$  and  $l$  results in a frequency  $\nu=(E_u-E_l)/h$ . The absorption line will be described by a line profile function  $\Phi(\nu)$  which is peaked and normalized:

$$\int_0^\infty \Phi(\nu) d\nu = 1 \quad (2)$$

If the intensity of the radiation field is  $I_\nu$ , we can define an average intensity by:

$$\bar{I} = \int_0^\infty I_\nu \Phi(\nu) d\nu \quad (3)$$

The probability of the absorption of a photon is  $B_{lu}\bar{U}$  such that the number of absorbed photons is  $n_l B_{lu}\bar{U}$  where  $\bar{U}=4\pi\bar{I}/c$  is the average energy density of the radiation field. Einstein found that in order to derive Planck's law, another emission process was needed:  $n_u B_{ul}\bar{U}$  that is the number of photons emitted by stimulated emission. If the system is in a stationary state, the number of absorbed and emitted photons must be equal:

$$n_u A_{ul} + n_u B_{ul}\bar{U} = n_l B_{lu}\bar{U} \quad (4)$$

We can express  $j_\nu$  and  $\alpha_\nu$  by:

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \Phi(\nu) \quad (5)$$

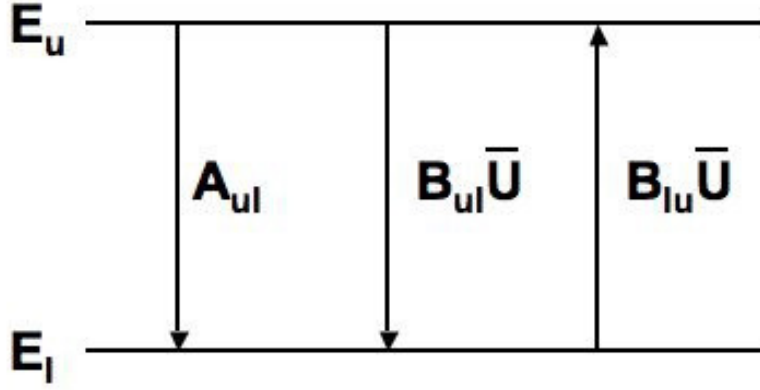


Figure 1: Transitions between the states up (u) and low (l) and the Einstein coefficients.

$$\alpha_\nu = \frac{h\nu}{c} (n_l B_{lu} - n_u B_{ul}) \Phi(\nu) \quad (6)$$

Let's define the opacity  $\tau$  of a line by :

$$d\tau = \alpha_\nu ds \quad (7)$$

and the source function by :

$$S_\nu = \frac{j_\nu}{\alpha_\nu} \quad (8)$$

Then we get :

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \quad (9)$$

$$\frac{dI_\nu}{d\tau_\nu} e^\tau + I_\nu e^\tau = S_\nu e^\tau \quad (10)$$

$$\frac{d}{d\tau_\nu} (I_\nu e^\tau) = S_\nu e^\tau \quad (11)$$

We can then integrate this equation between 0 and  $\tau_\nu$  :

$$\int_0^{\tau_\nu} \frac{d}{d\tau_\nu} (I_\nu e^\tau) d\tau_\nu = \int_0^{\tau_\nu} S_\nu e^\tau d\tau_\nu \quad (12)$$

Assuming that the source function is constant, we then get :

$$I_\nu = S_\nu + e^{-\tau_\nu}(I_{\nu_0} - S_\nu) \quad (13)$$

where  $I_{\nu_0}$  represents the cosmic microwave background (CMB) at 2.7 K. The emitted intensity of an astronomical source is coupled to the CMB. In order to compare the intensity of the observed signal with the original intensity of the emitting source in absence of the intervening interstellar medium ( $I_\nu(0)$ ), we get :

$$I_{\nu_{obs}}(s) = I_\nu(s) - I_\nu(0) = (S_\nu(T) - I_\nu(0))(1 - e^{-\tau_\nu}) \quad (14)$$

With this equation, we assume that the source function does not vary as a function of the opacity, namely it does not vary throughout the cloud. The source function can be described as :

$$S_\nu = \frac{\frac{h\nu}{4\pi} n_u A_{ul}}{\frac{h\nu}{c} (n_l B_{lu} - n_u B_{ul})} \quad (15)$$

We can describe an excitation temperature,  $T_{ex}$ , which characterizes the population levels :

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-\frac{h\nu}{kT_{ex}}} \quad (16)$$

Then :

$$S_\nu = \frac{A_{ul} c}{4\pi} \frac{1}{\frac{g_l}{g_u} e^{E_{ul}/kT_{ex}} B_{lu} - B_{ul}} \quad (17)$$

In LTE, the brightness distribution is described by the Planck function, which depends only on the thermodynamic temperature  $T$  of the surroundings (blackbody radiation) :

$$S_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \quad (18)$$

$$I_\nu(0) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/2.7k} - 1} \quad (19)$$

From equations 17, 18 and 19, we find that the Einstein coefficients  $A_{ul}$ ,  $B_{ul}$  and  $B_{lu}$  are not independent and must obey :

$$g_l B_{lu} = g_u B_{ul} \quad (20)$$

$$A_{ul} = \frac{8\pi h\nu^3}{c^3} B_{ul} \quad (21)$$

We note that the previous equation defines  $B$  in terms of radiation density per unit frequency interval. The intensity of radiation at frequency  $\nu$ , observed by a telescope, is given by :

$$I_{obs} = (I(T_{ex}) - I(T_{CMB}))(1 - e^{-\tau_\nu}) \quad (22)$$

where  $T_{ex}$  is the excitation temperature in the cloud and  $T_{CMB}$  is the cosmic microwave background at 2.7 K. In the Rayleigh-Jeans limit (namely  $\frac{T_0}{T} \ll 1$  where  $T_0 = h\nu/k$ ),

$$I_\nu = \frac{2kT}{\lambda^2} \quad (23)$$

It is the custom in radioastronomy to measure the brightness of a source by its brightness temperature,  $T_b$ . This is the temperature which would result in the given brightness if inserted into the Rayleigh-Jeans law.

Equation 22 then becomes :

$$T_b(v) = T_0 \left( \frac{1}{e^{T_0/T_{ex}} - 1} - \frac{1}{e^{T_0/2.7} - 1} \right) (1 - e^{-\tau(v)}) \quad (24)$$

where  $T_0 = h\nu/k$ .

When a background continuum source ( $T_{dust}, \tau_{dust}$ ) is coupled to the molecular/atomic cloud ( $T_{ex}, \tau$ ) along the line of sight, the previous equation must take into account the dust temperature and opacity, as well as the cosmic microwave background (CMB). In a on-off observation, the resulting brightness temperature obtained from the telescope is :

$$T_b = J_\nu(CMB)e^{-\tau_{dust}}e^{-\tau} + \Omega_{dust}J_\nu(T_{dust})(1 - e^{-\tau_{dust}})e^{-\tau} + \Omega J_\nu(T_{ex})(1 - e^{-\tau}) - J_\nu(CMB) \quad (25)$$

where  $J_\nu(T) = (h\nu/k) * 1/(e^{h\nu/kT} - 1)$  is the radiation temperature,  $\Omega_{dust}$  represents the dilution factor for the continuum source and  $\Omega$  represents the dilution factor for the molecular/atomic cloud. In the case where  $\tau_{dust} = 0$  and  $\Omega = 1$ , the equation becomes :

$$T_b = (J_\nu(T_{ex}) - J_\nu(CMB))(1 - e^{-\tau}) \quad (26)$$

In the case where  $\Omega = \Omega_{dust} = 1$ , then:

$$T_b = (J_\nu(CMB)e^{-\tau_{dust}} + J_\nu(T_{dust})(1 - e^{-\tau_{dust}}))e^{-\tau} + T_{ex}(1 - e^{-\tau}) - J_\nu(CMB) \quad (27)$$

Outside the line, towards the continuum source, the continuum obtained in the on-off observation is defined by:

$$T_C = (J_\nu(CMB)e^{-\tau_{dust}} + J_\nu(T_{dust})(1 - e^{-\tau_{dust}})) - J_\nu(CMB) \quad (28)$$

Combining equations 27 and 28 give a resulting brightness temperature that is used for the CASSIS formalism :

$$T_b = T_C e^{-\tau} + (1 - e^{-\tau}) (J_\nu(T_{ex}) - J_\nu(CMB)) \quad (29)$$

- For emission lines:

$$T_b - T_C = \Delta T = (1 - e^{-\tau}) (J_\nu(T_{ex}) - J_\nu(CMB) - T_C) \quad (30)$$

- For absorption lines:

$$T_C - T_b = T_{abs} = (1 - e^{-\tau}) (T_C - J_\nu(T_{ex}) + J_\nu(CMB)) \quad (31)$$

Several components (spatially distributed, with different  $V_{LSR}$  and/or temperature/density) and molecules can be modelled at the same time. For each molecules, several transition can be modelled within the spectrum. The spectra of these components are computed separately, and then added iteratively. In the following equations, the indices i, j and k correspond to components, molecules, and lines, respectively. The spectrum is computed in a first iteration with the first component:

$$T_{b,0}(\nu) = I_C(\nu) e^{-\sum_{j,k} \tau_{0,j,k}(\nu)} + \sum_j \eta_{0,j} \left( 1 - e^{-\sum_k \tau_{0,j,k}} \right) (J_\nu(T_{ex,0,j,k}) - J_\nu(T_{bg})) \quad (32)$$

where  $\eta$  is the beam dilution factor lying between 0 and 1 (see Section VI). The other components are then added iteratively:

$$T_{b,i=[1,N-1]}(\nu) = T_{b,0}(\nu) e^{-\sum_{j,k} \tau_{i,j,k}(\nu)} + \sum_j \eta_{i,j} \left( 1 - e^{-\sum_k \tau_{i,j,k}} \right) (J_\nu(T_{ex,i,j,k}) - J_\nu(T_{bg})) \quad (33)$$

The continuum emission is assumed to be optically thin (i.e. transparent to the CMB) and spatially uniform, to fill the beam of the single-dish telescope or the synthesized beam of the interferometer. For the moment, it is not possible to use a beam dilution for the continuum within CASSIS.  $T_{bg}$  should have the same value along the same line of sight, for all modelled components. In LTE,  $T_{ex,i,j,k}$  has the same value within each component (i) for each transition (k).

The line opacity can be expressed as a function of the column density and the excitation temperature, that we assume to be constant on the line of sight :

$$\int \tau dv = \int \frac{h\nu\Phi_\nu}{c} (B_{lu}n_l - B_{ul}n_u) dv = \frac{g_u}{g_l} \frac{A_{ul}c^3 n_l}{8\pi\nu^3} (1 - \exp(-h\nu/kT_{ex})) \quad (34)$$

Where  $\Phi_\nu$  is the line profile with  $\int \Phi(\nu) d\nu = 1$ .

For a gaussian line shape, we can express the opacity as a function of the cloud's depth :

$$\tau_{ul}(z) = \frac{A_{ul}c^3}{8\pi\nu_{ul}^3 \Delta v \sqrt{\pi}/2\sqrt{\ln 2}} \int_0^z n_u \left( \frac{n_l g_u}{n_u g_l} - 1 \right) dz' \quad (35)$$

where  $\Delta v$  (velocity units) is the full width at half maximum of the observed line. Integrating on the line of sight, we get, at the line center :

$$\tau_0 = \frac{g_u}{g_l} \frac{c^2}{8\pi\nu^2 \Delta\nu \sqrt{\pi}/2\sqrt{\ln 2}} A_{ul} N_l \left(1 - e^{-h\nu/kT_{ex}}\right) \quad (36)$$

where  $\Delta\nu$  (frequency units) is the full width at half maximum of the observed line, and  $N_l$  is the column density in the lower state.

This equation can also be expressed as:

$$\tau_0 = \frac{c^2 A_{ul} N_u}{8\pi\nu^2 \Delta\nu \sqrt{\pi}/2\sqrt{\ln 2}} \left(e^{h\nu/kT_{ex}} - 1\right) \quad (37)$$

This can be related to the total column density:

$$N_{tot} = N_{lowest} Q(T_{ex}) / g_{lowest} = N_u Q(T_{ex}) e^{E_u/kT_{ex}} / g_u. \quad (38)$$

where  $Q(T_{ex})$  is the partition function for an excitation temperature  $T_{ex}$  and the index "lowest" represents the lowest level associated to the molecule and its form (ortho, para, ...).  $E_u$  is the upper level of the transition compared to the ground level (different from zero when ortho, para or meta forms). When the collision rate between molecules is high (in LTE),  $T_{ex} \rightarrow T_b \rightarrow T_K$ . By choosing a column density such that  $\tau \gg 1$  at the line center, the line will therefore saturate, the temperature at the line center will become constant, and will result in a non-negligible line broadening (see Equation 24). At  $T_{ex} = 20$  K, for the  $^{12}\text{CO}$  molecule, we get  $T_b = 16.5$  K for the  $1 \rightarrow 0$  transition and  $T_b = 14.8$  K for the  $2 \rightarrow 1$  transition. Figure 2 presents the line profiles of the  $^{12}\text{CO}$  molecule for transitions  $1 \rightarrow 0$  and  $2 \rightarrow 1$  at  $T_{ex} = 20$  K, FWHM = 1 km s $^{-1}$ ,  $\tau = 10$  and  $\tau = 0.5$  at the line center.

Several mechanisms can broaden spectral lines. The most important involves the Doppler effect. Individual atoms are in random, chaotic motion. The hotter the gas, the faster the random thermal motions of the atoms. When a photon is emitted by an atom in motion, the frequency of the detected photon is changed by the Doppler effect. The photon is then not recorded at the precise frequency predicted by atomic physics but rather at a slightly shifted. Throughout the whole cloud, atoms move in every possible direction, resulting in a broadening of the line. From Fuller & Myers (1992) :

$$(\Delta v)^2 = 8 \ln(2) \frac{kT}{m} \quad (39)$$

where  $\Delta v$  is the full width at half maximum,  $k$  is the Boltzmann constant,  $T$  is temperature in the gas, and  $m$  is the mass of the atom (or molecule). For example,



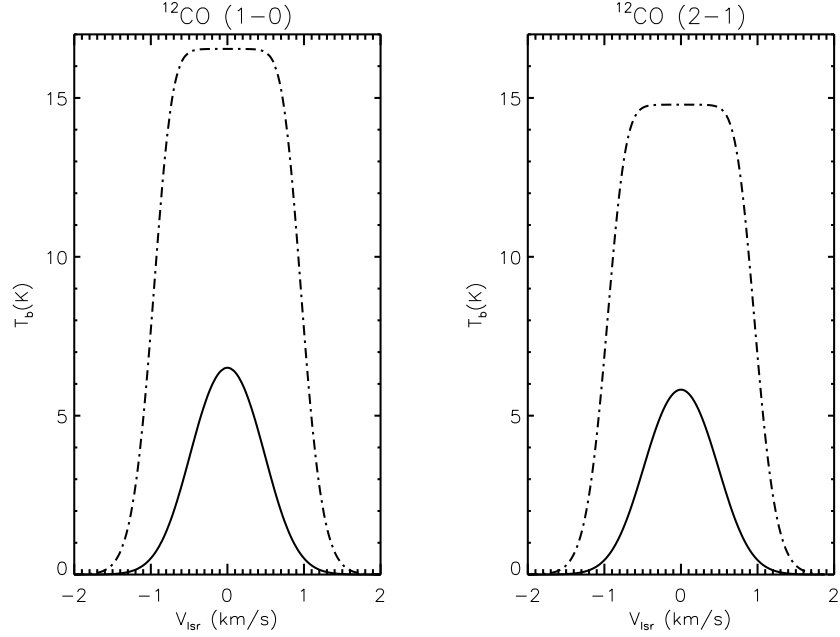


Figure 2: Line profiles for the  $^{12}\text{CO}$  transitions  $1 \rightarrow 0$  and  $2 \rightarrow 1$  at  $T_{ex} = 20$  K,  $\Delta v = 1$  km s $^{-1}$  and  $\tau = 0.5$  (plain lines) and 10 (dot-dashed lines) at the line center.

in the case of the  $\text{D}_2\text{H}^+$  molecule, at a temperature of 8 K, the thermal linewidth will be 0.27 km/s. Note that turbulence can also result in the broadening of a spectral line.

**For CASSIS:** by defining a column density and an excitation temperature, we get from 34  $\int \tau dv$ . Then, using a linewidth (before broadening due to optical depth), we get  $\tau(v)$  (as a function of velocity), which has a gaussian profile:

$$\tau(v) = \tau_0 \exp\left(-\frac{(v - v_0)^2}{2\sigma^2}\right) \quad (40)$$

where  $v_0$  is the velocity in the local standard of rest ( $V_{LSR}$ ),  $\sigma$ (km/s) =  $\Delta v$ (km/s)/( $2\sqrt{2\ln 2}$ ), where  $\Delta v$  is the full-width at half maximum. Then from 24 we get  $T_b$  as a function of velocity. This results in a line profile that is to be included in CASSIS.

## II. Use of a non-LTE radiative transfer code within CASSIS: RADEX

You can also use a non-LTE radiative transfer code within the CASSIS software. RADEX is a statistical equilibrium radiative transfer code and is made available for public use as part of the Leiden Atomic and Molecular Database (LAMDA). It is a one-dimensional non-LTE radiative transfer code, that uses the escape probability formulation assuming an isothermal and homogeneous medium without large-scale velocity fields. RADEX is comparable to the LVG method and provides a useful tool in rapidly analyzing a large set of observational data providing constraints on physical conditions, such as density and kinetic temperature.

If you plan to use RADEX within CASSIS, you have first to download, install and check RADEX :

- Download RADEX from the official RADEX website: <https://personal.sron.nl/~vdtak/radex/index.shtml>
- Install and check RADEX as stated on the RADEX website
- When your RADEX install is working, copy the whole RADEX directory into your current CASSIS directory. This is mandatory because CASSIS will change some files of RADEX, making it unusable outside CASSIS. Do not run RADEX standalone from the RADEX directory in CASSIS, run it from your original install directory. Note that the collisional files in the RADEX/Data directory are not used, as used with RADEX standalone. CASSIS will use the collisional files in its database/lamda directory.

The input parameters are: the kinetic temperature, the density of the collision partner ( $\text{H}_2$ ,  $\text{p-H}_2$ ,  $\text{o-H}_2$ , electrons, H (atoms), He, and  $\text{H}^+$ ), the molecular column density, the line width and the temperature of background radiation (2.73 K by default). RADEX computes the opacity of the line, the excitation temperature (K), the peak intensity (K) and the line flux (K.km/s) which is simply calculated as the integral of the Gaussian:  $\int T_R dv = T_R \times FWHM \times \frac{\sqrt{2\pi}}{2\sqrt{2\ln(2)}}$  where FWHM is the Full Width at Half Maximum (km/s).

The integrated profile is useful for estimating the total amount of emission in the line, although it has limited meaning for optically thick lines since the changing optical depth over the profile is not taken into account. Using the RADEX code as a standalone version, the entire radiative transfer is performed with rectangular line shapes.

Here is an example of the output from RADEX standalone on the HCO<sup>+</sup> molecule:

Radex version : 30nov2011

Geometry : Uniform sphere

Molecular data file : /Users/vastel/CODES/Radex/data/hco+.dat

T(kin) [K]: 100.000

Density of H2 [cm-3]: 1.000E+11

T(background) [K]: 2.730

Column density [cm-2]: 3.000E+14

Line width [km/s]: 1.000

Calculation finished in 10 iterations

Line	$E_{up}$	Freq(GHz)	$T_{ex}$ (K)	$\tau$	$T_R$ (K)	Flux(K.km/s)
2-1	12.8	178.3748	100.0	1.814E+00	7.985E+01	8.500E+01
3-2	25.7	267.5573	100.0	3.670E+00	9.122E+01	9.710E+01
4-3	42.8	356.7338	100.0	5.618E+00	9.132E+01	9.721E+01
5-4	64.2	445.9024	100.0	7.245E+00	8.961E+01	9.539E+01

CASSIS uses the opacity and excitation temperature from the output file, to reconstruct the line profile using equation 29. For optically thick lines, CASSIS will broaden the line profile although RADEX keeps a constant FWHM. Linewidths may be different from one line to another due to the opacity effect, therefore one computation for one unique FWHM cannot be done.

For example, Fig. 3 shows a synthetic spectrum of the 5-4 transition of HCO<sup>+</sup> (black line=LTE model with 8 K noise) for the above parameters ( $N=3 \times 10^{14} \text{cm}^{-2}$ , FWHM= 1 km/s,  $T_{ex}=100$  K). We perform the RADEX modeling (red line) using a high density so that we reach LTE ( $n_{H_2} = 10^{11} \text{cm}^{-3}$ ), with  $T_k = 100$  K. Using a 1km/s line width, the integrated flux intensity from RADEX should be 95.39 K.km/s (see table above), well below the observed flux of  $\sim 1.8$  (km/s)  $\times 89.6$  (K)= 161.3 K.km/s, where 1.8 km/s represents the line width of the observed line (after broadening due to the opacity effect). Using a 1.8 km/s line width in the standalone RADEX version gives:

Line	$E_{up}$	Freq(GHz)	$T_{ex}$ (K)	$\tau$	$T_R$ (K)	Flux(K.km/s)
5- 4	64.2	445.9024	100.0	4.025E+00	8.807E+01	1.688E+02

with a line flux of 168.8 K.km/s compatible with the modelled flux from CASSIS.

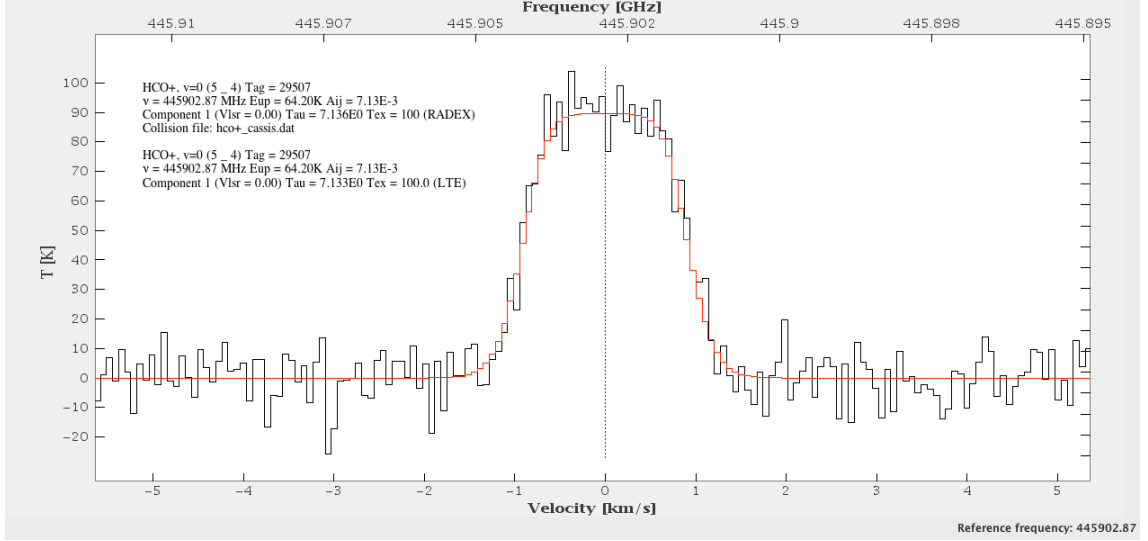


Figure 3: Modeled HCO<sup>+</sup> 5-4 transition in LTE (black) and with RADEX (red).

### III. Molecules (using the JPL or CDMS catalogs)

#### 1) The Einstein $A_{ul}$ coefficients

The line intensity in the catalogs,  $I_{ul}(300K)$  is obtained from:

$$I_{ul}(T) = \frac{8\pi^3}{3hc} \nu_{ul} S_{ul} \mu^2 [e^{-E_l/kT} - e^{-E_u/kT}] / Q_{rs}(T) \quad (41)$$

where  $\nu_{ul}$  is the line frequency,  $S_{ul}$  is the line strength,  $\mu$  is the dipole moment along the molecular axis and  $Q_{rs}$  is the rotation-spin partition function (using the same zero of energy as  $E_u$  and  $E_l$ ). The units of intensity given in the catalog is  $\text{nm}^2 \cdot \text{MHz}$ . The average spontaneous emission rate from the upper states into the lower states is:

$$A_{ul} = I_{ul}(T) \nu_{ul}^2 \frac{Q_{rs}(T)}{g_u} \frac{1}{e^{-E_l/kT} - e^{-E_u/kT}} \times \frac{8\pi}{c^2} \quad (42)$$

where  $T = 300$  K.

$$A_{ul} = I_{ul}(T) \nu_{ul}^2 \frac{Q_{rs}(T)}{g_u} \frac{1}{e^{-E_l/kT} - e^{-E_u/kT}} \times 2.796410^{-16} \text{ s}^{-1} \quad (43)$$

where  $I_{ul}(T)$  is in  $\text{nm}^2 \cdot \text{MHz}$  and  $\nu$  is in MHz.

#### 2) The partition functions

In the cold regions of the ISM it is important to consider ortho and para states separately. The energy of the lowest rotational or rotation-hyperfine level is 0 by default. The energy of the lowest level for the other spin-modification(s) is usually given in the documentation. One should consider Q values for the different spin-modifications separately at least at low temperatures. The CDMS database intends to provide this information in the near future.

In the CASSIS database, the new catalog (tagged "VASTEL") takes into account the ortho/para/A/E forms for the H<sub>2</sub>O, D<sub>2</sub>O, H<sub>2</sub>S, D<sub>2</sub>S, H<sub>2</sub>CO, CH<sub>3</sub>OH, H<sub>2</sub><sup>13</sup>CO, H<sub>2</sub>C<sup>18</sup>O, D<sub>2</sub>CO, NH<sub>3</sub>, NH<sub>2</sub>D, CH<sub>3</sub>CCH, HCOOCH<sub>3</sub>, c-C<sub>3</sub>H<sub>2</sub>, H<sub>2</sub>D<sup>+</sup> and D<sub>2</sub>H<sup>+</sup> molecules. The JPL catalog has been used for the NH<sub>3</sub>, D<sub>2</sub>S, H<sub>2</sub>O, D<sub>2</sub>O, c-C<sub>3</sub>H<sub>2</sub>, CH<sub>3</sub>OH, HCOOCH<sub>3</sub> and H<sub>2</sub>S molecules; the CDMS catalog has been used for the NH<sub>2</sub>D, H<sub>2</sub>CO, H<sub>2</sub><sup>13</sup>CO, H<sub>2</sub>C<sup>18</sup>O, D<sub>2</sub>CO, D<sub>2</sub>O, D<sub>2</sub>S, H<sub>2</sub>S, H<sub>2</sub>O, CH<sub>3</sub>CCH, c-C<sub>3</sub>H<sub>2</sub>, H<sub>2</sub>D<sup>+</sup> and D<sub>2</sub>H<sup>+</sup> molecules.

A file called catdir.cat is also provided. Each element of this file has the following format:

TAG: the species tag or molecular identifier (8 or 9 on the 5th digit to separate the ortho/para/A/E symmetry). For example 020091 for o-D<sub>2</sub>O, means that the CDMS catalog (original D<sub>2</sub>O = 020502) has been used (4th digit) to be compared with 20592 for o-D<sub>2</sub>O where the JPL database has been used (original D<sub>2</sub>O tag= 020001).

NAME: an ASCII name for the species.

NLINE: the number of lines in the catalog.

QLOG: A seven-element vector containing the base 10 logarithm of the partition function for temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, 9.375 K, respectively. The main interest of having those Q(Tex) for each symmetry, is an accurate computation for the column density for a symmetry state, or in the case of CASSIS, computation of the main beam temperature for a line of a certain symmetry.

VERSION: the version of the calculation for this species in the catalog (starts at number 69).

ALOG: the base 10 logarithm of the partition function for temperature of 300 K as found in the CDMS or JPL database, where the ortho and para forms are not disentangled. **This value is necessary to compute the Einstein coefficients.**

Note that the partition functions are provided at temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, 9.375 K. Interpolation is made for temperatures inside this range. So LTE model for lower temperatures (e.g. 6 K) can be problematic. However, CASSIS provides also the computation for lower temperatures than

9.375 K and higher than 300 K for many species. The files are provided in the cassis/database/sqlPartitionMole directory as ascii files. If you plan to make a LTE model outside the usual range [9.375-300] K, you should check whether your species is in this directory. For example, in the case of the para  $c\text{-C}_3\text{H}_2$  molecule, you can check that the file 38582.txt file in the cassis/database/sqlPartitionMole has a computed partition function as low as 3 K, with a value 2.3 times lower than the value at 9.375 K. By default, CASSIS will use the partition functions provided in this directory.

### example 1: $\text{H}_2\text{O}$ and $\text{D}_2\text{O}$

$\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  are asymmetric top molecules, with the dipole moment along the b-axis. They have ortho and para forms. The notation for the transitions is  $J, K_a, K_c$ .

For  $\text{H}_2\text{O}$ :

$g_J = 3(2J+1) \Sigma K$  odd : ortho transitions  
 $g_J = (2J+1) \Sigma K$  even : para transitions  
 $Q_{para}(T_{ex}) = \Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$  where  $E_{0-para} = 0$  K  
 $Q_{ortho}(T_{ex}) = \Sigma g_i e^{-(E_i - E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 34.23$  K  
1113342.9640 0.3000 -0.8353 3 0.0000 3 -180031404 1 1 1 0 0 0 0 0  
556936.0020 0.0500 -0.8147 3 23.7944 9 -180031404 1 1 0 0 1 0 1 0

For  $\text{D}_2\text{O}$ :

$g_J = 6(2J+1) \Sigma K$  even : ortho transitions  
 $g_J = 3(2J+1) \Sigma K$  odd : para transitions  
 $Q_{para}(T_{ex}) = \Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$  where  $E_{0-para} = 17.43$  K  
 $Q_{ortho}(T_{ex}) = \Sigma g_i e^{-(E_i - E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 0$  K  
607349.6000 0.2000 -1.3353 3 0.0000 18 -20001 303 1 1 1 0 0 0  
316799.8100 0.1200 -2.0408 3 12.1170 9 -20001 303 1 1 0 1 0 1

### example 2: $\text{H}_2\text{S}$ and $\text{D}_2\text{S}$

The  $\text{H}_2\text{S}$  and  $\text{D}_2\text{S}$  molecules are asymmetric top molecules. They have ortho and para forms. The notation for the transitions is  $J, K_a, K_c$ .

For  $\text{H}_2\text{S}$ :

$g_J=3(2J+1)$   $\Sigma K$  odd : ortho transitions  
 $g_J=2(2J+1)$   $\Sigma K$  even : para transitions  
 $Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$  where  $E_{0-para} = 0$  K  
 $Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 19.78$  K  
452390.3300 0.0700 -2.6154 3 0.0000 3 -34002 303 1 1 1 0 0 0  
168762.7624 0.0100 -2.8376 3 13.7463 9 -34002 303 1 1 0 1 0 1

For D<sub>2</sub>S:

$g_J=6(2J+1)$   $\Sigma K$  even : ortho transitions  
 $g_J=3(2J+1)$   $\Sigma K$  odd : para transitions  
 $Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$  where  $E_{0-para}=10.01$  K  
 $Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 0$  K  
91359.1209 0.0230 -4.1358 3 6.9561 9 340 303 1 1 0 1 0 1  
237903.6752 0.0581 -3.1702 3 0.0000 18 340 303 1 1 1 0 0 0

### example 3: H<sub>2</sub>CO and D<sub>2</sub>CO

H<sub>2</sub>CO and D<sub>2</sub>CO are planar asymmetric top molecules but the asymmetry is very small: they are therefore almost prolate symmetric top molecules with the dipole moment along the A-axis. The notation for the transitions is J,K<sub>a</sub>,K<sub>c</sub>.

For H<sub>2</sub>CO:

$g_J=(2J+1)$  K<sub>a</sub> is even : para transitions  
 $g_J=3(2J+1)$  K<sub>a</sub> is odd : ortho transitions  
 $Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$  where  $E_{0-para}=0$  K  
 $Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 15.16$  K  
4829.6600 .0010 -5.9024 3 10.5390 9 -30004 303 1 1 0 1 1 1  
72837.9480 .0100 -4.1792 3 .0000 3 -30004 303 1 0 1 0 0 0

Then:

$$Q_{tot}(T_{ex}) = Q_{para}(T_{ex}) + e^{-15.16/T_{ex}} Q_{ortho}(T_{ex})$$

For D<sub>2</sub>CO:

$g_J=6(2J+1)$  K<sub>a</sub> is even : ortho transitions

$g_J=3(2J+1)$   $K_a$  is odd : para transitions  
 $Q_{para}(T_{ex})=\sum g_i e^{-(E_i-E_{0-para})/kT_{ex}}$  where  $E_{0-para} = 8.05$  K  
 $Q_{ortho}(T_{ex})=\sum g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$  where  $E_{0-ortho} = 0$  K  
 6096.0673 .0039 -6.2883 3 5.5983 9 32006 303 1 1 0 1 1 1  
 58468.6700 .1000 -4.1897 3 .0000 18 -32006 303 1 0 1 0 0 0

#### example 4: $H_2D^+$ and $D_2H^+$

These molecules are asymmetric top molecules. The notation for the transitions is  $J, K_a, K_c$ .

For  $D_2H^+$ :

$g_I=6(2I+1)$   $\Sigma K$  even : ortho transitions (warning: different from the documentation file in the CDMS catalog)

$g_I=3(2I+1)$   $\Sigma K$  odd : para transitions (warning: different from the documentation file in the CDMS catalog)

The partition function for the ortho transitions will be different than the one for the para transitions. This is necessary in order to estimate the main beam temperature from a column density of a line or to determine the column density from an observation. The need is all the more important as the energy difference between the zero level for the ortho transitions and the zero level for the para transitions is large (see Figure 4).

$$Q_{para}(T_{ex})=\sum g_i e^{-(E_i-E_{0-para})/kT_{ex}}$$

$$Q_{ortho}(T_{ex})=\sum g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$$

where  $E_{0-para}$  is the fundamental energy of the para level (50.2 K) and  $E_{0-ortho}$  is the fundamental energy of the ortho level (0 K).

$Q_{para}(T_{ex}=8K)=9.1$	$Q_{ortho}(T_{ex}=8K)=6.00$
$Q_{para}(T_{ex}=10K)=9.3$	$Q_{ortho}(T_{ex}=10K)=6.02$
$Q_{para}(T_{ex}=12K)=9.6$	$Q_{ortho}(T_{ex}=12K)=6.05$
$Q_{para}(T_{ex}=15K)=10.0$	$Q_{ortho}(T_{ex}=15K)=6.16$

For  $H_2D^+$ :

$g_I=3(2I+1)$   $K_a$  odd : ortho transitions

$g_I=1(2I+1)$   $K_a$  even : para transitions

$$Q_{para}(T_{ex})=\sum g_i e^{-(E_i-E_{0-para})/kT_{ex}}$$

$$Q_{ortho}(T_{ex})=\sum g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$$



where  $E_{0-para}$  is the fundamental energy of the para level (0 K) and  $E_{0-ortho}$  is the fundamental energy of the ortho level (86.4 K).

$$\begin{aligned} Q_{para}(T_{ex}=8\text{K}) &= 1.00 \\ Q_{para}(T_{ex}=10\text{K}) &= 1.00 \\ Q_{para}(T_{ex}=12\text{K}) &= 1.01 \\ Q_{para}(T_{ex}=15\text{K}) &= 1.04 \end{aligned}$$

$$\begin{aligned} Q_{ortho}(T_{ex}=8\text{K}) &= 9.96 \\ Q_{ortho}(T_{ex}=10\text{K}) &= 10.51 \\ Q_{ortho}(T_{ex}=12\text{K}) &= 11.03 \\ Q_{ortho}(T_{ex}=15\text{K}) &= 11.74 \end{aligned}$$

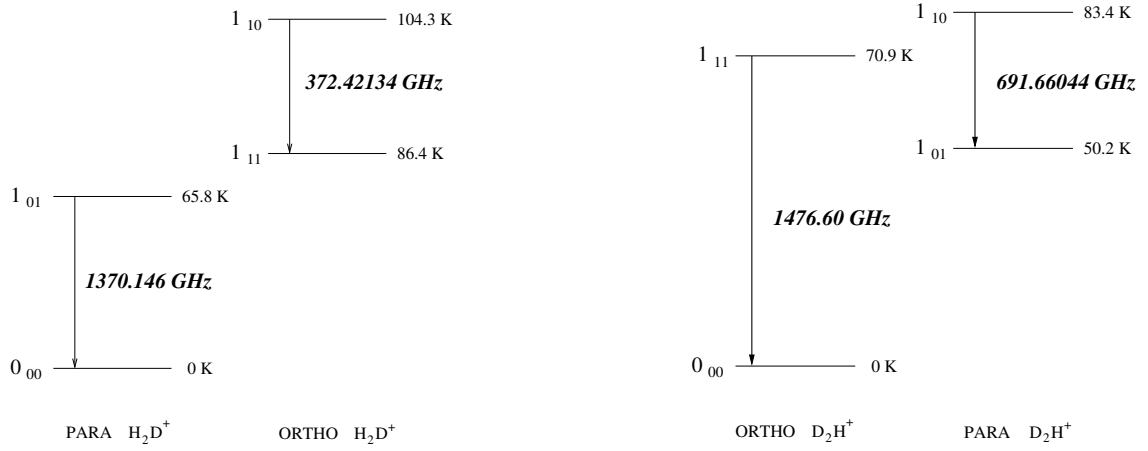


Figure 4: Lower energy transitions for the  $\text{H}_2\text{D}^+$  and  $\text{D}_2\text{H}^+$  molecules.

## IV. Absorption lines

### 1) Astrophysical observations

The determination of column densities from absorption lines is more accurate in general, with respect to the quantities inferred from the analysis of emission lines, because the calculated value does not depend on the excitation temperature of the line,  $T_{ex}$ , as long as this is negligible with respect to the temperature of the background continuum source  $T_c$ .

$$N_{\text{tot}} = \frac{8\pi\nu^3}{A_{ul}c^3} \Delta\nu \frac{\sqrt{\pi}}{2\sqrt{\ln 2}} \frac{g_l}{g_u} \tau_0 \quad (44)$$

and,

$$\tau_0 = -\ln\left(1 - \frac{T_{\text{abs}}}{T_C}\right) \quad (45)$$

where  $\tau_0$  is the opacity at the line center,  $T_{\text{abs}}$  is the temperature of the absorption line and  $T_C$  is the temperature of the continuum. The opacity profile is defined as 40. Using  $T(v)$  (with the 0 K level reference) we get  $T(v) = T_C - T_{\text{abs}}(v)$ . Absorption lines can then be determined (see Figure 5).

CASSIS take into account the background continuum and the excitation temperature of the lines (see section I) to determine the line intensity (see equation 29):

$$T_b = T_C e^{-\tau} + (1 - e^{-\tau}) (J_\nu(T_{\text{ex}}) - J_\nu(\text{CMB})) \quad (46)$$

Since  $N_{\text{tot}}$  can be computed as (see section I):

$$N_{\text{tot}} = \frac{8\pi\nu^3}{A_{ul}c^3} \Delta\nu \frac{\sqrt{\pi}}{2\sqrt{\ln 2}} \frac{\tau_0 Q(T_{\text{ex}})}{g_u} \frac{\exp(E_u/kT_{\text{ex}})}{[\exp(h\nu/kT_{\text{ex}}) - 1]} \quad (47)$$

then, the opacity is deduced and therefore the line profile. NB:  $E_u$  is the upper level of the transition compared to the ground level (different from zero when ortho, para or meta forms).

Towards SgrB2(M), we get a continuum of  $\sim 1920$  Jy around 692 GHz in a 30" beam and  $\sim 4000$  Jy around 1476 GHz in a 20" beam (Goldsmith, Lis, Hill, Lasenby 1990). The HIFI beam width is  $\sim 30''$  at 692 GHz and  $\sim 13''$  at 1476 GHz. The conversion from source flux density to antenna temperature is:

$$S_\nu(\text{Jansky}) = T_a(\text{K}) / (\eta\pi D(\text{cm})^2 / 8k) = 3520 \times \frac{T_A(\text{K})}{\eta_A(D(\text{meters}))^2}$$

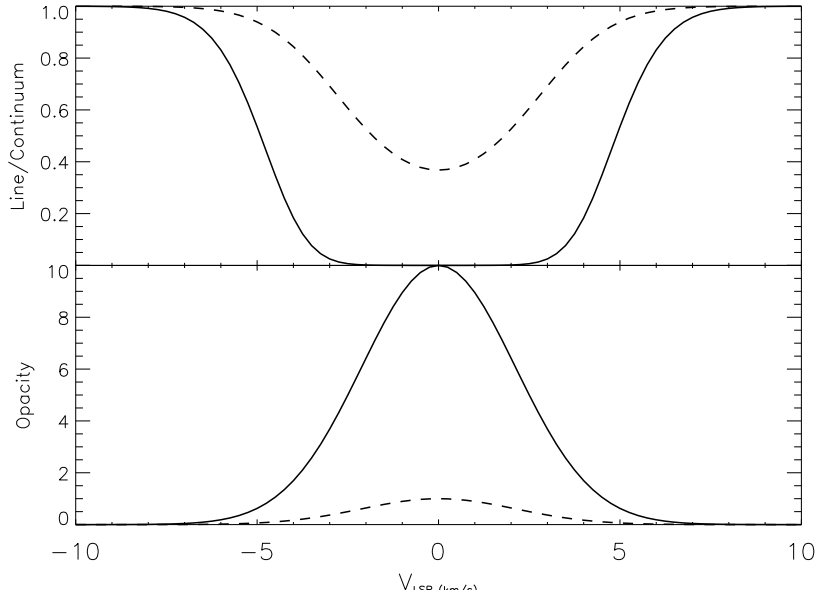


Figure 5: Example of absorption lines. The upper plot represents 2 absorption features with an opacity of 10 (plain line) and with an opacity of unity (dashed-line), with a linewidth of  $5 \text{ km s}^{-1}$  and a continuum normalized to unity. The lower plot represent the opacity profiles for the same lines.

This corresponds, for the Herschel dish diameter of 3.5 m, to a continuum of about 5 K at 692 GHz and  $\sim 10$  K at 1476 GHz.

For a  $1.3 \cdot 10^{13} \text{ cm}^{-2}$   $\text{D}_2\text{H}^+$  column density, with FWHM=1 km/s, we get:

- 1) at 691 GHz,  $\tau \sim 0.2$  and  $\frac{T_{\text{abs}}}{T_C} \sim 0.2$
- 2) at 1476 GHz,  $\tau \sim 0.36$  and  $\frac{T_{\text{abs}}}{T_C} \sim 0.3$

## 2) Laboratory measurements: gas cells

The informations concerning the physical conditions in the environment can be deduced from the shape of the observed lines. There are several cause of line broadening, the main being:

Natural broadening: The Uncertainty principle relates the life of an excited state with the precision of the energy, so the same excited level will have slightly different energies in different atoms. This broadening effect is described by a Lorentzian profile.

Thermal Doppler broadening: Atoms will have different thermal velocities, so they will see the photons red or blue shifted, absorbing photons of different energies in the frame of reference of the observer. The higher the temperature of the gas, the larger the velocity differences (and velocities), and the broader the line. This broadening effect is described by a Doppler profile.

Pressure broadening: the collision of other particles with the emitting particle interrupts the emission process. The duration of the collision is much shorter than the lifetime of the emission process. This effect depends on the density of the gas. The broadening effect is described by a Lorentzian profile.

Opacity broadening: considerable reabsorption of emission line photons, an effect known as opacity, often causes line broadening. The line is broadened since photons at the line wings have a smaller reabsorption probability than photons at the line center (see previous section).

The combined line profile will be the convolution of the line profiles of each mechanism. For example, a combination of thermal Doppler broadening and pressure broadening will yield a Voigt profile. The natural broadening is usually too small to be taken into account. the Voigt profile must be evaluated by numerical integration.

Let's consider a Lorentzian profile  $f_L$  and a Gaussian profile  $f_G$ . The resulting line shape will result in a Voigt profile  $f_V$ , which can be expressed as the convolution of the first two:

$$f_\nu(\nu - \nu_0, \delta\nu_L, \delta\nu_D) = f_L \otimes f_G = \frac{\sqrt{\ln 2} a}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{[-(\ln 2)(\nu' - \nu_0)^2 / \delta\nu_D^2]}{(\nu - \nu')^2 + \delta\nu_L^2} d\nu' \quad (48)$$

where  $\delta\nu_L$  and  $\delta\nu_D$  are half-widths of the Lorentzian and Gaussian profiles respectively,  $\nu$  is the source frequency,  $\nu_0$  is the frequency of the line center and  $a$  is the ratio of the profiles width ( $\delta\nu_L/\delta\nu_D$ ). We used the Liu et al. (2001) empirical analytical approximation to determine the Voigt profile:

$$f_V(\nu - \nu_0, \delta\nu_V) = c_L f_L(\nu - \nu_0, \delta\nu_V) + c_G f_G(\nu - \nu_0, \delta\nu_V) \quad (49)$$

$$= c_L \frac{1}{\pi} \frac{\delta\nu_V}{(\nu - \nu_0)^2 + \delta\nu_V^2} + c_G \frac{\sqrt{\ln 2}}{\sqrt{\pi} \delta\nu_V} \exp\left(\frac{-(\ln 2)(\nu - \nu_0)^2}{\delta\nu_V^2}\right) \quad (50)$$

From Olivero and Longbothum (1977, J. Quant. Spectrosc. Radiati. Transfer):

$$\delta\nu_V = 0.5346\delta\nu_L + \sqrt{0.2166\delta\nu_L^2 + \delta\nu_D^2} \quad (51)$$

Introducing a dimensionless parameter,  $d=(\delta\nu_L-\delta\nu_D)/(\delta\nu_L+\delta\nu_D)$ , the weight coefficients are given by:

$$c_L = f_1(d) , \quad c_G = f_2(d) \quad (52)$$

where  $d$  is the profile parameter. If  $d=1$  ( $-1$  respectively), we obtain a pure Lorentz profile (Gaussian respectively).

Liu et al. (2001) found from the fitting on 2 molecules that:

$$c_L = 0.68188(17) + 0.61293(31) \times d - 0.18384(39) \times d^2 - 0.11568(44) \times d^3 \quad (53)$$

$$c_G = 0.32460(17) - 0.61825(31) \times d + 0.17681(39) \times d^2 + 0.12109(44) \times d^3 \quad (54)$$

The pressure broadening can be obtained from the HITRAN database. After selecting the molecule and the spectral range you need, the JavaHAWKS software will produce a file output. This file is read by CASSIS as "File output from HITRAN". The  $\gamma_{self}$  parameter (in  $\text{cm}^{-1}.\text{atm}^{-1}$  at 296 K) is then extracted and converted for the needed temperature  $T$  and pressure  $P$ .

$$\delta\nu_L = \gamma_{self} \times \frac{P(\text{mbar})}{1013.25} \times 299792.45810^5 \times \frac{T}{296} \quad (55)$$

The probability that a molecule in a gas at temperature  $T$  has a velocity  $v$  in a particular direction is proportional to  $\exp(-mv^2/2kT)$ , where  $m$  is the molecular mass. Consequently the line is symmetric and has a half width at half maximum of:

$$\delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2(\ln 2)kT}{m}} \quad (56)$$

Determining the line profile, the absorption coefficient  $\alpha_{max}$  (in units of  $\text{cm}^{-1}$ ) can be obtained from  $I_{ba}$ :

$$\alpha_{max}[L^{-1}] = H[L^2] \times n[L^{-3}] \quad (57)$$

where  $H$  is the line strength,  $L$  is the length of the gas cell and  $n$  is the density in the gas cell ( $=P/kT$ ).  $H$  can be expressed as a function of  $I_{ba}$  (in  $\text{nm}^2.\text{MHz}$ ; based on the integral of the absorption cross-section over the spectral line shape: see figure 6):

$$I_{ba} = H \times \left[ \pi\delta\nu_L + \sqrt{\frac{\pi}{\ln 2}}\delta\nu_D \right] \quad (58)$$

Then, we get:

$$\alpha_{max} = H \times n = \frac{I_{ba}}{\pi\delta\nu_L + \sqrt{\frac{\pi}{\ln 2}}\delta\nu_D} \times \frac{P}{kT} \quad (59)$$

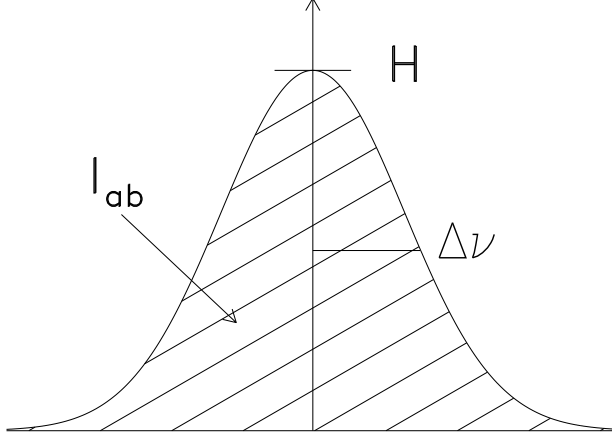


Figure 6: Gaussian line profile, with height  $H$ , and half width at half maximum  $\delta\nu$  and the integrated profile represented by the  $I_{ab}$  parameter (in  $\text{nm}^2.\text{MHz}$ ) from the JPL and CDMS catalogues.

The power transmission through a uniform medium of length  $L$  at the peak of the line is  $\exp(-\alpha_{max}L)$ . The opacity can be computed as  $\alpha_{max}L$ .

Example:  $^{12}\text{CO}$  (4-3) transition at 461040.7682 MHz, in a 102.54 cm length cell, at  $T=300$  K, and  $P=3.3$  mB<sup>1</sup>. From the HITRAN database  $\delta\nu_L = 7451480.17$  Hz. At  $T=300\text{K}$   $\delta\nu_D = 1076200.38$  Hz.

$$\alpha_{max} = \frac{10^{-3.2657}}{(\pi\delta_L + \sqrt{\frac{\pi}{\ln 2}}\delta_D) \times 3.02284} \times \frac{3.310^3}{1.3810^{-16} \times 300} \times 10^{-18} \times 10^{-2} \quad (60)$$

The opacity is then about  $0.018 \text{ cm}^{-1} \times 102.54 \text{ cm}=1.83$ . In Figure 7 we present a comparison between the laboratory measure and the result from a convolution between a Gaussian profile (thermal Doppler broadening) and a Lorentzian profile (pressure broadening) assuming that the opacity is equal to . We see that we can't reproduce the observed profile with the given parameters.

<sup>1</sup>1 bar =  $10^6$  baryes, 1 mmHg = 0.00133 bar, 1 Torr = 1mm Hg, 760 mm Hg = 101325 Pa=1 atm=1013.25 mbar. The cgs unit for pressure is barye (1 mB =  $10^3$  barye).

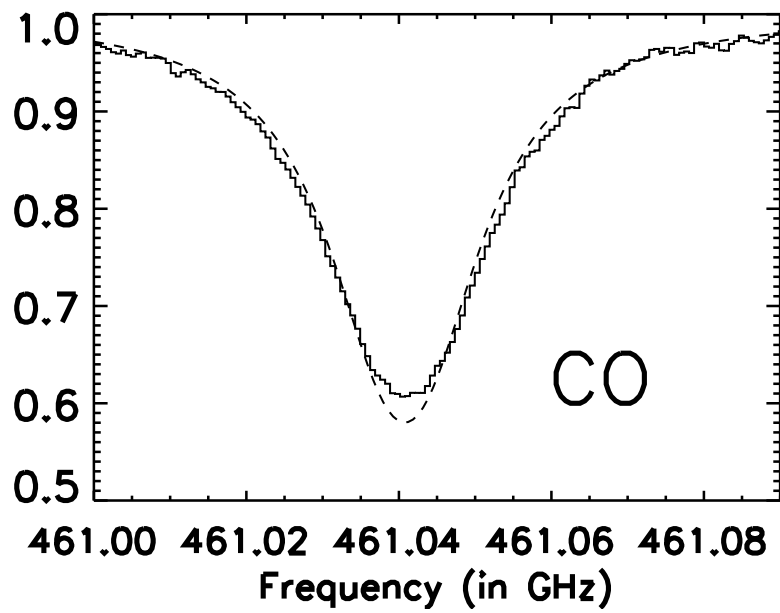


Figure 7: Comparison between the observed HIFI spectrum (plain line) and the modeled line using the conditions in the gas cell (dashed-line).

## V. Rotational diagram (population diagram analysis)

This term refers to a plot of the column density per statistical weight of a number of molecular energy levels, as a function of their energy above the ground state (see Goldsmith and Langer 1999). In LTE, this corresponds to a Boltzmann distribution, so a plot of the natural logarithm of  $N_u/g_u$  versus  $E_u/k$  yields a straight line with a slope of  $1/T_{rot}$ . The temperature inferred represents the rotation temperature. From Chapter I., we can write the optical depth of the transition as:

$$\tau = \frac{c^3 A_{ul} N_u}{8\pi\nu^3 \Delta\nu \sqrt{\pi}/2\sqrt{\ln 2}} [e^{h\nu/kT_{rot}} - 1] \quad (61)$$

Neglecting the 2.7 K radiation ( $h\nu/k \gg 2.7$ ), we can express the main beam temperature as:

$$T_b = \frac{h\nu}{k} \frac{1}{\exp(h\nu/kT_{rot}) - 1} \frac{1 - e^{-\tau}}{\tau} \times \tau \quad (62)$$

Therefore, we can compute the column density in the upper state as:

$$N_u = \int T_b dv \times \frac{8\pi k\nu^2}{hc^3 A_{ul}} \times \frac{\tau}{1 - e^{-\tau}} \quad (63)$$

$$N_u = W \times \frac{8\pi k\nu^2}{hc^3 A_{ul}} \times C_\tau \quad (64)$$

Where  $W$  in the integrated area and  $C_\tau$  is the optical depth correction factor. When the line is optically thin,  $C_\tau$  is equal to unity.

For a molecule in LTE, all excitation temperatures are the same, and the population of each level is given by:

$$N_u = \frac{N_{tot}}{Q(T_{rot})} g_u e^{-E_u/kT_{rot}} \quad (65)$$

We can rewrite this equation to obtain:

$$\ln \frac{N_u}{g_u} = \ln \frac{N_{tot}}{Q(T_{rot})} - \frac{E_u}{kT_{rot}} \quad (66)$$

A rotational diagram can be useful to determine whether the emission is optically thick or thin, whether the level populations are described by LTE, and to determine what temperature describe the population distribution in the event that LTE applies. Equation 66 can be written in terms of the observed integrated area  $W$ :

$$\ln \frac{8\pi k\nu^2 W}{hc^3 A_{ul} g_u} = \ln \frac{N_{tot}}{Q(T_{rot})} - \ln C_\tau - \frac{E_u}{kT_{rot}} \quad (67)$$



If we don't take into account the  $C_\tau$  factor, each of the upper level populations would be underestimated by a factor  $C_\tau$ , different for each transition. Therefore, the ordinate of the rotation diagram would be below its correct value by the factor  $\ln C_\tau$ . A change in the temperature for lines of different excitation might indicate that the source has different temperature components or that the lines considered are not optically thin and cannot be easily used to obtain a meaningful excitation temperature.

Note that the error bars should be taken into account for the order 1 polynomial fit, in order to obtain a reliable value for the uncertainty on the rotational temperature as well as the total column density. From the Line Analysis module the user can fit the lines and CASSIS produces a detailed .rotd file with the integrated area and rms values for each transitions. The user is required to give a value for the instrumental calibration uncertainty. The uncertainty of the integrated area is therefore computed through the following formula:

$$\Delta W = \sqrt{(\text{cal}/100 \times W)^2 + (\text{rms}\sqrt{2} \times \text{fwhm} \times \Delta v)^2} \quad (68)$$

where cal is the calibration value (%),  $W$  is the integrated area (in K km/s), rms is the noise around the selected species (in K), fwhm is the full width at half maximum (km/s) and  $\Delta v$  is the bin size (in km/s). Therefore, the plotted uncertainties are simply:

$$\Delta \left( \ln \frac{N_u}{g_u} \right) = \frac{\Delta W}{W} \quad (69)$$

Now, how do we estimate the uncertainty on the values of  $T_{rot}$  and  $N_{tot}$ ?

From the fitted straight line ( $y = ax+b$ ) the slope  $a$  is related to the rotational excitation temperature as  $T_{rot} = -1/a$ . Then  $\Delta T_{rot} = \Delta a/a^2$ . The intercept  $b$  is related to the total column density as  $N_{tot} = Q(\text{rot}) \times e^b$ . Therefore  $\Delta N_{tot} = Q(\text{rot}) \times \Delta b \times e^b$ .

We can iteratively apply the  $C_\tau$  correction to the rotational diagram analysis until a solution for  $T_{rot}$  and  $N_{tot}$  has converged (convergence to be defined in CASSIS in % for the value of epsilon). For the first iteration we use Equation 66 and obtain values for the transitions opacity. In the second iteration we add the  $C_\tau$  correction to the linear equation:

$$\ln \frac{N_u}{g_u} = \ln \frac{N_{tot}}{Q(T_{rot})} - \frac{E_u}{kT_{rot}} - \ln C_\tau \quad (70)$$

The iterations go on until a convergence has been obtained.

As Goldsmith and Langer (1999) nicely said, this method requires quite a large number of transitions spread over a range of upper state energies.

CASSIS provides the values for the column density, excitation temperature and the corresponding errors, reduced  $\chi^2$  and the probability of occurrence (P value) for a  $\chi^2$  value depending on degrees of freedom. The degree of freedom in our linear fit corresponds to the number on points (n) on which the fit was performed minus 2 (2 values extracted from the fit: N and  $T_{ex}$ ).

The method of least squares states that the best values are those for which S is minimized:

$$S = \sum_{i=1}^n \frac{(y_i - y)^2}{\sigma^2} = \sum_{i=1}^n \frac{(y_i - ax_i - b)^2}{\sigma_i^2} \quad (71)$$

Ideally S is expected to follow a chi-square distribution with its mean value equal to the degrees of freedom "dof". We thus expect S to be close to dof = n - 2 if the fit is good. A quick and easy test is to form the reduced chi-square  $\chi^2/\text{dof}$  which should be close to 1 for a good fit. A more rigorous test is to look at the probability of obtaining a  $\chi^2$  value greater than S, i.e.,  $P(\chi^2 \geq S)$ . This requires integrating the  $\chi^2$  distribution or using cumulative distribution tables. In general, if  $P(\chi^2 \geq S)$  is greater than 5%, the fit can be accepted. This probability is just a tool for deciding whether to reject or validate the fit as frequentist statistics does not, and cannot, attach probabilities to hypotheses. An important point to consider is when S is very small. This implies that the points are not fluctuating enough. Beyond falsified data, the most likely cause is an overestimation of the errors on the data points. Indeed, the error bars represent a 1  $\sigma$  deviation, so that about 1/3 of the data points should be expected to fall outside the fit. If the errors have been under-estimated then an improbably high value of  $\chi^2$  can be obtained.

CASSIS provides the reduced  $\chi^2$  and the probability  $P(\chi^2 \geq S)$ . Values of the  $\chi^2$  or reduced  $\chi^2$  corresponding to the probability  $P(\chi^2; \text{dof}=2)$  of exceeding  $\chi^2$  can be found in the literature (e.g. "Data reduction and error analysis for the physical sciences", Bevington, Robinson, McGraw-Hill, 2003). Since the true probability of the data being consistent with the model depends on both  $\chi^2$  and dof, we decided to provide the reduced  $\chi^2$  and the probability so that the user decides on the goodness of its fit. For example, if we obtain a value of  $\chi^2 = 1.95$  for 7 degrees of freedom, the corresponding probability is about 96%. Although this probability may seem to be gratifyingly high, the very low value of  $\chi^2$  gives a strong indication that the common uncertainty in the data may have been overestimated.

If you plan on performing a population diagram analysis on 2 points only, CASSIS will evidently not be able to provide the errors on the column density and excitation temperature nor the  $\chi^2$  and probability values.

Note that CASSIS can perform the rotational diagram analysis assuming optically thin lines for multiplet transitions ( $\sim$  same frequency,  $\sim$  same upper energy), but not on blended transitions ( $\sim$  same frequency, different upper energy). However the opacity correction cannot be performed on both for the moment.

After using the Rotational Diagram module within CASSIS, I suggest that you use the column density and excitation temperature values in the Line Analysis module in order to compare the synthetic spectrum with your observations.

## VI. Telescopes parameters

By defining the flux density per beam as  $S_{\nu,b} = K \times S_{\nu,tot}$  (K being the correction factor: Baars 1973) we get:

$$S_{\nu,b} = \frac{2kT'_A}{A_{eff}} \quad (72)$$

where  $T'_A$  is the antenna temperature, only corrected for atmospheric losses:

$$T'_A = T_A \exp(-\tau_z A) \quad (73)$$

where  $\tau_z$  is the opacity at the zenith, and A is the air mass ( $1/\sin(\text{elevation})$ ). It can be converted into antenna temperature ( $T_A^*$ ), corrected for atmospheric attenuation, the forward efficiency and the signal band gain:

$$T'_A = T_A^* \times F_{eff} \quad (74)$$

where  $F_{eff}$  is the forward efficiency. The main beam temperature is then the temperature of an equivalent source just filling the main beam:

$$T_{mb} = \frac{F_{eff}}{B_{eff}} T_A^* = \frac{T'_A}{B_{eff}} \quad (75)$$

In equation 72,  $A_{eff}$  is the effective antenna area defined by the product between the aperture efficiency  $\eta_A$  and the geometrical area of the aperture,  $A_{geom} = \pi(D/2)^2$  where D is the diameter of the telescope.  $\eta_A$  is the ratio of the strength of the signal received from a point source to that which would have been received by a telescope of the same diameter that had no losses or blockage, having uniform illumination, and no surface errors.

Then equation 72 becomes:

$$S_{\nu,b} = \frac{2kT_{mb}B_{eff}}{\eta_A \pi(D/2)^2} \quad (76)$$

in  $\text{erg/s/cm}^2/\text{Hz}$ . Note that  $1 \text{ Jansky} = 10^{-23} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$ .

To compare with flux in  $\text{erg/s/cm}^2$ , we have to multiply this equation by  $\Delta\nu = \Delta v \times \nu/c$ .

$$Flux(\text{erg/s/cm}^2) = \frac{2kT_{mb}B_{eff}}{\eta_A \pi(D/2)^2} \times \Delta v \times \frac{\nu}{c} \quad (77)$$

Which means that:

$$T_{mb} \Delta v = Flux(\text{erg/s/cm}^2) \times \frac{\pi(D/2)^2}{2k} \times \frac{c}{\nu} \times \frac{\eta_A}{B_{eff}} \quad (78)$$

Another way to compute it is using the Rayleigh-Jeans approximation:

$$B_\nu = \frac{2\nu^2}{c^2} \Omega k T_{mb} \quad (79)$$

$$B_\nu = \frac{2k}{\lambda^3} \Omega \int T_{mb} dv \quad \text{in } erg/s/cm^2 \quad (80)$$

Then:

$$\int T_{mb} dv = Flux(erg/s/cm^2) \times \frac{c^3}{\nu^3} \times \frac{1}{2k\Omega} \quad (81)$$

For HIFI, with an effective aperture of 3.28 m:

- 1) telescope aperture efficiency = 64 % at 1.9 THz and 72 % at 500 GHz leading to a conversion factor of 511 Jy per Kelvin (in  $T_a^*$ ) at 1.9 THz, and 454 Jy per Kelvin (in  $T_a^*$ ) at 500 GHz.
- 2) telescope main beam efficiency =  $\sim 90$  % leading to a conversion factor of 460 Jy per Kelvin (in  $T_{mb}$ ) at 1.9 THz, and 408 Jy per Kelvin (in  $T_{mb}$ ) at 500 GHz..

CASSIS uses the concept of beam dilution. The beam filling factor (ff) is the fraction of the telescope beam occupied by the source. The observed intensity is reduced by the beam filling factor ( $T_{mb} = T_b \times ff$ ). A filling factor of unity means that the source is much larger than the beam. For distant clouds or external galaxies the filling factor is less so beam filling corrections are needed. For Gaussian source and beam it can be expressed as:

$$ff = \frac{\Omega_{source}}{\Omega_{observed}} \quad (82)$$

We assume for single dish observations, that the telescope beam FWHM size is related to the diameter of the telescope by the diffraction limit:

$$\theta = 1.22\lambda/D \quad (83)$$

where  $\theta$  is the angular resolution (radians),  $\lambda/$  is the wavelength of light, and D is the diameter of the telescope. The gaussian beam is frequently used in formula deduction for single dish. The size of a gaussian beam is characterized by FWHM of the power pattern:  $\theta_b$ . Then solid angle of such a gaussian beam is:

$$\Omega_b = \int \exp[-4\ln 2 \times \theta^2/\theta_b^2] \times 2\pi \times \theta d(\theta) = \frac{\pi}{4 \times \ln 2} \times \theta_b^2 = 1.133 \times \theta_b^2 \quad (84)$$

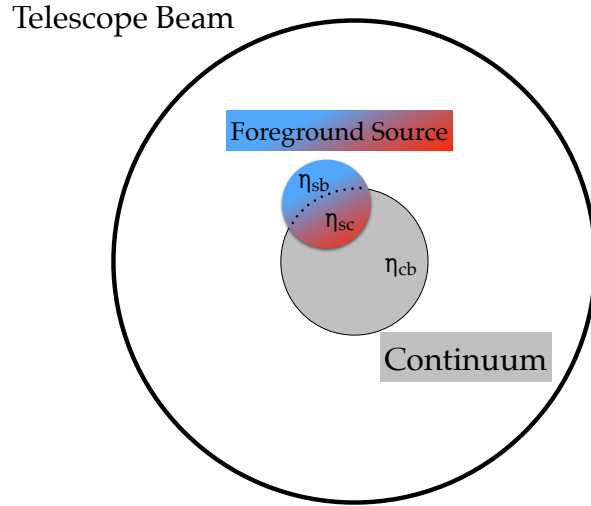
Therefore, the filling factor can be expressed as:

$$ff = \frac{\theta_{source}^2}{\theta_{source}^2 + \theta_{beam}^2} \quad (85)$$

Figure 8 shows a sketch of a possible geometry: the background continuum source fills part of the telescope beam (filling factor  $\eta_c$ ); the clumpy foreground source covers part of the continuum source (filling factor  $\eta_{sc}$ ), and partly extends over the beam area outside of the continuum source (filling factor  $\eta_{sb}$ ). The observed brightness temperature is then:

$$T_b = (1-\eta_{cb})(J_\nu(T_{cmb})+\eta_{sb}(1-e^{-\tau})(J_\nu(T_{ex})-J_\nu(T_{cmb}))) + \eta_{cb}(T_c - \eta_{sc}(1-e^{-\tau})(J_\nu(T_{ex})-T_c)) \quad (86)$$

the first part of the equation being the emission outside the continuum and the second part being the emission inside de continuum. Note that in CASSIS we do not deal with the beam dilution of the continuum using the assumption that the beam covers the continuum ( $\eta_{cb}=1$ ). The equation is therefore equivalent with our equation 32.



$\eta_{cb}$ = filling factor of the continuum in the beam  
 $\eta_{sb}$ = filling factor of the fraction of the source outside the continuum in the beam  
 $\eta_{sc}$ = filling factor of the fraction of the source inside the continuum in the beam

Figure 8: Beam and source geometry.

## VI. References

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