

Radiation Bookkeeping: a guide to
astronomical molecular spectroscopy and
radiative transfer problems with an emphasis
on **RADEX**

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1 Introduction

This document discusses some terminology necessary to extract chemical/physical information from spectral line observations. Although this is all very basic material, there are at least two astronomers who were often confused about these things. This little guide discusses quantities like brightness temperatures, antenna temperatures, beam dilution, line centre optical depth, flux density, Sobolev approximation, excitation temperature, column density.

The general goal is to give the practical steps to compare observations with some types of model calculations. The RADEX software is one of the simplest methods to constrain abundances and physical conditions from observations, and often serves as a useful guideline for using more complex radiative transfer programs. This document tries to explain what assumptions are implicitly made in RADEX, what else can be done, and how we compare this with our data.

The notation generally follows that used in Rybicki & Lightman (1), chapter 1, and Elitzur (2), chapter 2.

2 Basic radiative transfer

2.1 Fluxes and intensities

We start by defining the necessary quantities. This is most easily done in terms of energy. When a certain amount of energy is received at the telescope, it makes sense to divide these ergs by observing time, collecting area and bandwidth in order to be able to compare with somebody else who has a smaller telescope (but more observing time). So we define flux density:

$$F_\nu = \frac{dE}{d\nu dA dt}$$

Some people tend to call this simply flux, but flux is defined as $F = \int F_\nu d\nu$. Flux density is often expressed in Jansky ($1 \text{ Jy} = 1 \cdot 10^{-23} \text{ erg cm}^{-2} \text{ Hz}^{-1}$).

The flux F is straightforwardly connected to the source luminosity by

$$F = \frac{L}{4\pi D^2}$$

where D is the distance to the object. So we have a direct expression of the energy production of our source. This is, however, of limited use as it does not tell us anything about densities, temperatures and chemical abundances, especially when we deal with line radiation that may saturate. To get this

information, we have to follow the radiative transfer of separate spectral lines. This is most easily done by using intensities.

Intensities are defined as

$$I_\nu = \frac{dE}{d\nu dA dt d\Omega \cos\theta}.$$

In fact, we should call I_ν the specific intensity to make a distinction with I , but most people however refer to I_ν when they use the word intensity. Here Ω is the solid angle the source subtends and θ equals the angle between dA and the ray for which we measure I_ν . Most telescopes are designed cleverly enough to have this angle at 0° for a source in their field of view, so we can usually take $\cos\theta = 1$, but it is kept for consistency. This implies

$$F_\nu = \iint I_\nu \cos\theta d\Omega.$$

The difference between flux density and specific intensity is clearly illustrated when we study a source of radius R at distance D . Let's assume the source produces a constant amount of L_ν photons of interest at its surface. Then we already know

$$F_\nu = \frac{L_\nu}{4\pi D^2}$$

so that the flux is independent of the size of the source, but does depend on the distance to the object. However the intensity is

$$I_\nu = \frac{F_\nu}{\Delta\Omega} = \frac{L_\nu}{4R^2}$$

which depends on the true size of the object, but is now independent of the distance! Since the integral $\iint d\Omega = \pi$ we understand that the source intensity is $\pi F_{\nu,\text{surface}}$. The fact that I_ν is constant along a free travelling ray makes it easy to express radiative transfer in terms of intensity. But let's look at antenna temperatures first.

2.2 Antenna temperatures

The power received by the radio telescope from a source (in erg s^{-1}) can be expressed as

$$P^{\text{source}} = \frac{1}{2} A \eta_A (F_\nu^{\text{on}} - F_\nu^{\text{off}}) \Delta\nu$$

where the factor $\frac{1}{2}$ originates from the fact that we detect a single polarisation – see Kraus (3). We have subtracted out the background contribution. This power can be expressed in terms of the temperature of a resistor in

the telescope (and this is convenient as we can calibrate the telescope by switching on a hot load in the receiver).

$$P^{\text{source}} = k T_A \Delta\nu$$

(note that if we had not beam-switched this would define the T_{sys}). We can express T_A in terms of flux by working these formulas around. In general there are quite a number of steps to do this. For instance, the calibration of the atmospheric absorption leads to T'_A . There is quite some confusion about how different quantities are called – see Kutner & Ulich (4) for a consistent description. Without following all the details we denote $T_A/\eta_A = T_{\text{mb}}$ the main beam antenna temperature, which is also called T_R^* . This can now be related to the true T_R , the radiation temperature in the Rayleigh–Jeans approximation, if we know the quantitative effect of the beam convolution with the source. This depends not only on whether the source is resolved or not (see below) but also on how much radiation reaches the receiver through the sidelobes. Basically T_{mb} or T_R^* are as close as one can get to the radiation intensity without detailed knowledge about the beam of the telescope and the intensity distribution on the sky.

This main beam temperature is related to the flux observed by the telescope

$$T_{\text{mb}} = \frac{A}{2k} F_\nu^{\text{source}}.$$

where $F_\nu^{\text{source}} = F_\nu^{\text{on}} - F_\nu^{\text{off}}$. The telescope receives this power from a solid angle defined by the beam shape of the telescope. Let's define a solid angle $\Delta\Omega_A = \lambda^2/A$, then we can write this flux in terms of intensities.

For practical purposes it should be remembered that for a two dimensional gaussian beam holds

$$\Delta\Omega = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}} dy dx,$$

where we express the σ_x and σ_y in terms of FWHM Δ_x and Δ_y as

$$\sigma = \frac{\Delta}{2\sqrt{2 \ln 2}}$$

so we use

$$\Delta\Omega = (\Delta_x \Delta_y) \frac{\pi}{4 \ln 2}.$$

The intensities which will now be introduced should be used with caution. They are actually the *average* intensities over the beam. Only for resolved sources, these equal the source intensities, otherwise they are lower limits

to the source intensities. This fact that the inferred temperature is just a lower limit to the actual source brightness is called beam dilution. One could quantify this with a beam filling factor but we prefer

$$T_{\text{mb}} \leq \frac{c^2}{2\nu^2 k} I_{\nu}^{\text{source}}$$

or

$$T_{\text{mb}} \leq T_R,$$

where for a resolved source the equal sign holds and T_R is the Rayleigh–Jeans equivalent radiation temperature. Notice that the the Rayleigh–Jeans approximation is implicitly made above. So even in the regime where it does not hold, you will still get a RJ equivalent radiation temperature at the telescope. After we have discussed radiative transfer we will get back to this T_R and discuss its relation with the brightness temperature and the physical temperature of the emitting medium.

2.3 Radiative transfer

The fact that I_{ν} is constant along the line of sight makes it very easy to write radiative transfer in terms of intensity.

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

Other notations use for α_{ν} (the absorption coefficient in cm^{-1}) κ_{ν} ($=\alpha_{\nu}/\rho$ in $\text{cm}^2 \text{gr}^{-1}$, with ρ the mass density in gr cm^{-3}). Both are frequently expressed as $\alpha_{\nu} = n_i \sigma_{\nu}$ where σ_{ν} is the absorption cross section in cm^2 . Instead of j_{ν} one often finds ϵ_{ν} , the (volume) emission coefficient. Note that here it has already been assumed that the spontaneous emission is isotropic, i.e. does not depend on the direction we are studying. This is OK for spectroscopic purposes.

We can rewrite this equation by defining the optical depth $d\tau_{\nu} = \alpha(\vec{r})ds$ so that we can calculate the optical depth at a point s along the ray as

$$\tau_{\nu}(s) = \int_{s_0}^s \alpha(s') ds'.$$

Here optical depth is measured along the ray. Sometimes the minus sign of the radiative transfer equation is incorporated in the definition of τ_{ν} and then the optical depth is measured from the observer. For the τ_{ν} over the total depth of the source there is of course no difference.

Thus we can write the radiative transfer in the following form

$$\frac{dI_\nu}{d\tau} = -I_\nu + S_\nu(\vec{r}),$$

where the source function is the ratio of emission to absorption coefficient.

We can write the formal solution to this

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu) d\tau'_\nu.$$

Since we are interested in doing spectroscopy, let's write the α_ν and j_ν in terms of Einstein coefficients. A complication is that we have to worry about the line shape. For instance the Einstein A_{21} gives us how often spontaneous emission occurs from the upper (2) to the lower (1) level in a single atom, but we want to express j_ν in units of [erg cm⁻³ ster⁻¹ Hz⁻¹], because it is an intensity. So we write

$$j_\nu = \frac{h\nu_0}{4\pi} n_2 A_{21} \phi(\nu).$$

The 4π term is due to the assumption that the emission is isotropic, and $\phi(\nu)$ takes care of the line shape. It is a function for which must hold $\int \phi(\nu) d\nu = 1$. The most simple expression for $\phi(\nu)$, which is often used, is a rectangle of value $1/\Delta\nu$ and width $\Delta\nu$ around some $\nu = \nu_0(v_{\text{obs}}/c)$. Of course a gaussian profile is also often used, either with a width set by the kinetic temperature or a fixed velocity width which is assumed to be due to micro-turbulence. This discussion on $\phi(\nu)$ is rather trivial, but recall that one has to choose a $\phi(\nu)$ to calculate for instance an optical depth; usually the optical depth for the centre of the line is given. Also this is the place where peculiar line shapes due to internal motion are created.

For the absorption coefficient we find in a similar way

$$\alpha_\nu = \frac{h\nu}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu).$$

From considerations that the level populations must reach the Boltzmann distribution when the matter is in equilibrium with radiation in thermodynamic equilibrium (the Planck law) and the fact that this must hold even in the absence of collisional transitions, the Einstein relations can be derived:

$$g_1 B_{12} = g_2 B_{21}$$

and

$$A_{21} = \frac{2h\nu^3}{c^2} B_{21}.$$

With the expressions for j_ν and α_ν one can write the source function in terms of Einstein coefficients:

$$S_\nu = \frac{A_{21}}{B_{21}} \frac{1}{\frac{n_1 g_2}{g_1 n_2} - 1}.$$

We can define an excitation temperature which characterizes the ratio of n_1/n_2 :

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\frac{h\nu}{kT_{\text{ex}}}}$$

Taking this definition, the source function becomes

$$S_\nu = B_\nu(T_{\text{ex}}),$$

which makes an easy interpretation possible. Here $B_\nu(T)$ is the blackbody radiation field at temperature T :

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

The general solution for a homogeneous medium is

$$I_\nu = B_\nu(T_{\text{ex}})(1 - e^{-\tau_\nu}) + I_\nu^{\text{bg}} e^{-\tau_\nu}.$$

Insight can be obtained from the expression in the Rayleigh–Jeans approximation:

$$\frac{T_R}{d\tau_\nu} = -T_{\text{bg}} + T_{\text{ex}}.$$

I use the term T_R here, the radiation temperature and reserve T_B , brightness temperature, for $I_\nu = B_\nu(T_B)$, so only when the Rayleigh–Jeans approximation is accurate, $T_B = T_R$. A very simple transparent form is possible in a homogeneous medium

$$T_R = T_{\text{ex}}(1 - e^{-\tau_\nu}) + T_{\text{bg}} e^{-\tau_\nu}$$

One should realise that the excitation temperature describes only this single transition. In the case of thermal equilibrium, the n_1/n_2 population ratio is set by the Boltzmann function and the source function is the Planck function at T_{kin} .

3 Solving radiative transfer problems

3.1 Statistical equilibrium

The radiative transfer equation has been given in the last section, so the only problem left now is to specify some n_i to plug into the radiative transfer equation. This is where the problems arise. In principal we can write down the equation for statistical equilibrium; this is now just bookkeeping in which state our molecules (or atoms) are.

Before doing so, let's discuss collision rates. The rates C_{ij} are the collision rates per second per molecule of the species of interest. They must depend on the density of the collision partner, so they can be expressed as $C_{ij} = K_{ij}n^{\text{col}}$, where n^{col} the density of the collision partner is, often H_2 . The collisional rate coefficients K_{ij} (in $\text{cm}^3 \text{s}^{-1}$) are the velocity-integrated collision cross sections, and depend on temperature through the relative velocity of the colliding molecules and possibly also through the collision cross sections directly.

The collision rates obey the so-called detailed balance relations, which are the 'collisional analogs' to the Einstein relations. For a two-level system in thermodynamic equilibrium,

$$n_1 C_{12} = n_2 C_{21}$$

If we plug in the Boltzmann distribution for n_1 and n_2 with the appropriate statistical weights we find

$$C_{12} = \frac{g_2}{g_1} C_{21} e^{-\frac{\Delta E}{kT}}.$$

Since the K_{ij} are microscopical constants this relation must also hold in cases out of equilibrium.

Now we can write the statistical equilibrium down for the two level case (2,1).

$$\begin{aligned} \frac{dn_1}{dt} &= -n_1(B_{12}\bar{J} + C_{12}) + n_2(A_{21} + B_{21}\bar{J} + C_{21}) \\ \frac{dn_2}{dt} &= n_1(B_{12}\bar{J} + C_{12}) - n_2(A_{21} + B_{21}\bar{J} + C_{21}), \end{aligned}$$

where \bar{J} is J_ν integrated over $\phi(\nu)$, and J_ν is the average I_ν over the whole 4π steradian. To solve this we thus need to know the radiation field which was what we were after in the first place.

This problem can be solved, usually with some simplifying assumptions. I will discuss the escape probability method and the LTE assumption.

3.2 Escape probability

The problem is how to “decouple” the radiative transfer calculations from the calculations of the level populations. A popular approach for this is the escape probability method, first introduced by Sobolev (5) for expanding envelopes. The basic idea is to invent a factor that determines the chance that a photon at some position in the cloud can escape the system.

Remember that we need to estimate \bar{J} to calculate the level populations. Where does this intensity come from? It is the amount of radiation “inside” the source, so for a completely opaque source it equals the (profile averaged) source function S . If β is the chance that a newly created photon can escape from the cloud then $\bar{J} = S(1 - \beta)$. Now the statistical equilibrium equations take a very easy form:

$$\frac{dn_2}{dt} = n_1 C_{12} - n_2 C_{21} - \beta n_2 A_{21}.$$

So now we can solve the level populations and the radiation field separately; they are decoupled. In principle we can also easily add the contribution from background radiation here. We just take the background intensity, the average chance that it penetrates into the source is $(1 - \beta)$.

Now we are left with the task to estimate the escape probability. The method is based on the assumption that we can find some expression for this β depending on geometry and optical depth but not on the radiation field. Several forms have been proposed that depend on geometry; remember that we have to find a form that estimates the average local escape probability over all directions.

A very crude form of β in a one-dimensional case can be estimated as:

$$\beta = \langle e^{-\tau} \rangle = \frac{1}{\tau} \int_0^\tau e^{-\tau'} d\tau' = \frac{1 - e^{-\tau}}{\tau}.$$

In other expressions one usually expresses β in terms of the optical depth τ in the direction of the observer. It happens that the form of β for a radially expanding sphere is equal to the result above. This is called the Sobolev or large velocity gradient (LVG) approximation; see for example Elitzur (2), p. 44 for a derivation:

$$\beta = \frac{1 - e^{-\tau}}{\tau}$$

For a homogeneous slab is found:

$$\beta = \frac{(1 - e^{-3\tau})}{3\tau}$$

Also for a turbulent medium an escape probability has been estimated:

$$\beta = \frac{1}{\tau \sqrt{\pi \ln(\tau/2)}}$$

Finally for a uniform sphere, Osterbrock (6) derives

$$\beta = \frac{1.5}{\tau} \left[1 - \frac{2}{\tau^2} + \left(\frac{2}{\tau} + \frac{2}{\tau^2} \right) e^{-\tau} \right].$$

RADEX uses this last formula to estimate the excitation and radiation field in the following way. (For high optical depth, only the first term of the formula is retained; at low optical depth, a power series approximation is used.) As a first guess the level populations in the optically thin case (or for LTE) are calculated; this then gives the optical depth and hence the escape probability, from which the new level populations can be directly calculated. The program iterates this procedure to find a consistent level population and optical depth, and computes all line strengths for that solution. Practical details are given in the next section.

3.3 Optically thin radiation

We have seen that the problems with the coupling between radiation and level populations make a complex calculating scheme necessary. There are two limiting cases in which this complication disappears. First, when the radiation field in the *lines* is unimportant for the determination of the level populations, and second, when the level populations are in thermal equilibrium (LTE), although not necessarily in equilibrium with the radiation field (see next section).

Assuming that the level populations are not affected by radiation in the lines makes it possible to write all transition probabilities for the equations of statistical equilibrium, and you can solve directly the level populations. Thus one can calculate the line strengths from that. Note that for instance the $T_{\text{bg}} = 2.73$ K cosmic background radiation field always affects the lower level populations of heavy rotors like CO and CS. Because we assume the lines are optically thin we can easily take this into account.

3.4 Local Thermal Equilibrium

In local thermal equilibrium we assume that the level populations are governed by the Boltzmann equation and are thus independent of the radiation field. On Earth only in very special cases (e.g. inside lasers) does this assumption break down. But in most of the interstellar medium, the density

is so low that the populations are not thermalised and one can have natural maser phenomena. It can be important to make some estimate of the critical density for this process. For thermalisation, the time scale for collisions is significantly shorter than that for spontaneous decay. So we find

$$\frac{1}{C_{21}} \ll \frac{1}{A_{21}}$$

or

$$n \gg n_{\text{crit}}$$

where $n_{\text{crit}} = A_{21}/K_{21}$. This is readily reached for CO, where the Einstein coefficient is relatively low, giving $n_{\text{crit}} \approx 3 \cdot 10^3 \text{ cm}^{-3}$ for the $J=1 \rightarrow 0$ line, and implying that CO is a good thermometer. For other transitions, this is less easy. Take as an example HCO^+ $J=1 \rightarrow 0$ which has a critical density of $2 \cdot 10^5 \text{ cm}^{-3}$. Of course equilibrium is more easily established when the lines get optically thick, because the radiation will start to help the thermalisation of the levels.

In thermal equilibrium the source function becomes the Planck function, but in addition we can simplify the expression for the absorption coefficient, because we now know how the levels are populated. In LTE and a homogeneous medium

$$S_\nu = B_\nu(T)$$

and

$$\alpha_\nu = \frac{h\nu}{4\pi} n_1 B_{12} (1 - e^{-\frac{h\nu}{kT}}) \phi(\nu)$$

where the exponential term “corrects” for stimulated emission in the equilibrium assumption. The density of molecules in the lower state can be simply calculated from the Boltzmann distribution:

$$n_i = \frac{g_i e^{-\frac{E_i}{kT}}}{\sum_0^\infty g_j e^{-\frac{E_j}{kT}}} n_{\text{mol}}$$

When the source function is the Planck function it is illustrative to write the radiative transfer equation in terms of temperatures. This can only be done in the Rayleigh–Jeans limit because only then does the Planck function become linear (generally $B_\nu(T_1) + B_\nu(T_2) \neq B_\nu(T_1 + T_2)$). Taking the Rayleigh–Jeans limit of the transfer equation

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + B_\nu(T)$$

yields

$$\frac{T_R}{d\tau_\nu} = -T_R + T.$$

A simple solution is found for a homogeneous medium

$$T_R = T(1 - e^{-\tau_\nu}) + T_{\text{bg}}e^{-\tau_\nu}$$

So when the source is homogeneous, optically thick, and in LTE, $T_B = T$. Now if the Rayleigh–Jeans law holds then we know $T_B = T_R$. In § 2.2, it is shown that T_R is equal to the T_{mb} when the source is resolved. In summary, for an ideal telescope, looking at a resolved source with large optical depth ($\tau_\nu \gg 1$) which is in LTE ($n \gg n_{\text{crit}}$) we find for a line at the frequency where the Rayleigh–Jeans approximation holds that $T_A = T$.

4 RADEX

4.1 Input

The RADEX code was originally written by John Black, with improvements made in Leiden, and serves as a non-LTE excitation and radiative transfer code.

The first assumption in RADEX is that of a homogeneous medium. RADEX does not know anything about geometry or velocity fields. In particular it does not know whether the escape probability assumption holds. Because it does not know about source geometry one can specify the amount of material as a column density. The absence of knowledge of source structure also implies that RADEX cannot give a flux or specific luminosity, it can just produce intensities. This then implies that the user has to correct for beam dilution or make sure that the source is resolved. Often the easiest way out is obviously to try to model intensity ratios and hope/argue that the beam dilution for both lines is comparable. As resolution changes with telescope and observing frequency this is not easy.

The above drawbacks are (somewhat) compensated by the fact that it can deal with linear, symmetric-top and asymmetric-top molecules. It can model the collisional (de)excitations with up to seven different species and because the escape probability assumption has effectively decoupled the radiation from the molecular excitation it is possible to include background radiation.

To run the on-line version of RADEX, one needs to choose a molecular data file first. The format of these files is described on the Leiden molecular data

base homepage ¹. In addition, one must supply the following parameters:

- The spectral range for the output. This is only for convenience because some molecules have many lines and create lots of output. The calculations take all lines into account, of course
- The equivalent black body temperature of the background radiation field (usually taken to be the microwave cosmic background field, $T_{\text{CBR}}=2.73$ K)
- The kinetic temperature of the molecular cloud
- The number density of H₂ molecules in the cloud. The program can deal with other collision partners, but this is not implemented in the on-line version. Collisions with He are not taken into account; for a rough estimate, multiply the input density by 1.2 which is just the interstellar He abundance (He/H₂=0.2). The effects of mass and geometrical cross section between He and H₂ cancel out to first order.
- The ratio of ortho- to para-H₂ molecules in the cloud. This only matters for CO, H₂O and OH, where collisional rate coefficients exist for both types of H₂. Not sure what to do here? Just use the default value, which assumes that the H₂ $J=1/J=0$ ratio is thermalized at the kinetic temperature
- The column density of the molecule: this is the parameter to vary to match the output signal level
- The width of the molecular lines (assumed the same for all lines)

4.2 Calculation

Let's summarize the assumptions that are made. **RADEX** uses the escape probability method for a homogeneous medium. Furthermore we are blindly trusting somebody else's radiative and collisional transition rates. Note that the collision rates still depend on temperature. Such data are available for only a limited range of temperatures, and must therefore be interpolated or extrapolated. Notice that the relation $C_{12} = \frac{g_2}{g_1} C_{21} e^{-(\Delta E/kT)}$ ensures that for high densities the resulting distributions will go to their Maxwellian values, even if the rates are grossly wrong.

Also there are cases when one should worry whether a sufficient number of levels is taken into account, not just because collisions are exciting levels

¹<http://www.strw.leidenuniv.nl/~moldata> and/or
<http://www.mpifr-bonn.mpg.de/fvandertak/ratran/molformat.html>

that may not be present, but also because the ambient radiation field can excite higher levels (e.g., vibrational levels). In general, the data files are large enough to handle temperatures up to 500 K, but not much higher.

The calculations proceed as follows. A first guess of the relative populations of the levels is produced in the optically thin case. So background radiation is taken into account without being shielded, but no internally produced radiation is yet available. The solution for the level populations allows calculation of the optical depth in any of the lines, and thus we can find a new guess of the excitation by using the escape formalism. In this the background radiation is treated in exactly the same manner as the internally produced radiation. So we can iteratively find a consistent solution for the level populations and the radiation. The program decides when this has occurred and produces output.

The actual quantities and formulae that are used inside RADEX are as follows. The total intensity at line center frequency in $\text{erg s}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1}$ is given by

$$I_\nu^t = B_\nu(T_{\text{ex}}) [1 - e^{-\tau_0}] + e^{-\tau_0} I_\nu^b,$$

where the first term is the emission in the line and the second term the background emission at line frequency, reduced by any absorption in the line. The τ_0 is the optical depth at line centre. Both τ_0 and T_{ex} are calculated from the level populations (see below). $B_\nu(T)$ in convenient units is

$$B_\nu(T) = \frac{3.973 \times 10^{-16} \tilde{\nu}^3}{\exp(1.43883 \tilde{\nu}/T) - 1} \quad \text{ergs}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1},$$

where $\tilde{\nu}$ is the wave number in cm^{-1} .

The total intensity of the line in excess of background is:

$$I_\nu^t - I_\nu^b = (B_\nu(T_{\text{ex}}) - I_\nu^b) [1 - e^{-\tau}].$$

The brightness temperature T_B is defined as the temperature of a blackbody that would give the same intensity as that of a source of the same angular extent:

$$T_B = f(I_\nu^t) = \frac{1.43883 \tilde{\nu}}{\ln\left[\frac{3.973 \times 10^{-16} \tilde{\nu}^3}{I_\nu^t} + 1\right]} \quad \text{K}.$$

The brightness temperature of the line in excess of background is then given by

$$T_B = f(I_\nu^t) - f(I_\nu^b).$$

The Rayleigh–Jeans equivalent temperature T_R , which can be compared directly with observations, is given by

$$T_R = \frac{1}{2k\tilde{\nu}^2} (I_\nu^t - I_\nu^b).$$

The excitation temperature of a line, T_{ex} , is related to the ratio of populations of the two levels that participate in the transition $2 \rightarrow 1$:

$$\frac{x_2}{x_1} = \frac{g_2}{g_1} \exp\left[-\frac{E_2 - E_1}{k T_{\text{ex}}}\right],$$

where x_i is the fractional population in level i , g_i is the statistical weight of level i , and E_i the energy. The optical depth τ_0 in the line at line center is related to the populations by

$$\tau_0 = \frac{A_{21}}{8\pi\tilde{\nu}^3} \frac{\mathcal{N}}{\Delta v} \left[x_1 \frac{g_2}{g_1} - x_2\right],$$

where \mathcal{N} is the total column density of the molecule, and Δv is the FWHM of the line. Note that the optical depth, and therefore the RADEX results, only depend on the ratio of column density to line width, $\mathcal{N}/\Delta v$, which is similar to LVG programs.

In general, the background radiation is due to the $T_{\text{CBR}}=2.73$ K cosmic background radiation field and to far-infrared radiation by dust in the cloud with temperature T_d . The background intensity *seen by the observer* is then given by

$$I_\nu^b = B_\nu(T_{\text{CBR}}) + B_\nu(T_d)(1 - e^{-\tau_d}).$$

The background radiation in the cloud *seen by the molecules* may be diluted due to geometrical effects. If the lines are optically thin,

$$I_\nu^{b,\text{int}} = B_\nu(T_{\text{CBR}}) + \eta B_\nu(T_d)(1 - e^{-\tau_d}),$$

where η is a dilution factor lying between 0 and 1. If the lines are optically thick, the absorption and emission in the line itself modifies the internal radiation field in the escape probability formalism to

$$I_\nu^{\text{int}} = \beta \left[B_\nu(T_{\text{CBR}}) + B_\nu(T_d)(1 - e^{-\tau_d}) \right] + (1 - \beta) B_\nu(T_{\text{ex}}),$$

where β is the escape probability. This internal radiation field I_ν^{int} is used in the solution of the statistical equilibrium equations for the level populations x_i .

4.3 Results

In the on-line version of RADEX, the output pops up in a new window. After a repeat of the input parameters, you find for each spectral line in the range that you specified:

- the quantum numbers of the upper and lower states, which a format depending on the type of molecule
- the line frequency. For several molecules, the frequencies are of spectroscopic accuracy (0.1 MHz uncertainty), but please check up-to-date line catalogs² for the most precise values to use for observations
- the excitation temperature of that line. In general, different lines will have different excitation temperatures. Lines are thermalized if $T_{\text{ex}}=T_{\text{kin}}$; in the LTE case, *all* lines are thermalized.
- The optical depth at line center, calculated from $\phi(\nu) = 1/\Delta\nu$.
- TR, the Rayleigh–Jeans equivalent of the intensity of the line minus the background intensity. As discussed earlier, this is the quantity that is usually measured at the telescope.

The velocity-integrated intensity $\int T_R dv$ (also called line flux) can be calculated as $1.0645 T_R \Delta v$, where the factor 1.0645 ($\sqrt{\pi}/2\sqrt{\ln 2}$) is a correction to estimate the integration over a gaussian profile with FWHM of Δv compared to the adopted square profile. 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. In other words, the entire radiative transfer is performed with rectangular line shapes. Proper modeling of optically thick lines requires a program that resolves the sources both spectrally and spatially, using either the *Accelerated Lambda Iteration* or *Monte Carlo* method (see van Zadelhoff et al. (7) for a summary of methods and codes).

5 An example

It can be instructive to go through an example and calculate a few things and compare these with RADEX and “observations”. So let’s look at the CO $J=1\rightarrow 0$ emission from a small cloud, a uniform sphere in fact, with a diameter of 3000 AU, a temperature of 10 K and a total density of $n = 3 \cdot 10^3 \text{ cm}^{-3}$. We assume further that the fractional abundance of CO $f_{\text{CO}} = 8 \cdot 10^{-5}$, resulting in a CO column density of $\mathcal{N}_{\text{CO}} = 1.077 \cdot 10^{16} \text{ cm}^{-2}$.

The thermal line width of such a cloud is $\Delta v_{\text{kin}} = \sqrt{2kT/m_0} = 0.077 \text{ km/s}$. In most clouds the line widths are actually much broader than what we find from the temperature. It is assumed that the line width is set by

²<http://spec.jpl.nasa.gov> and/or <http://cdms.de>

microturbulence. Likewise I assume here $\Delta v = 1$ km/s, so $\Delta\nu = 0.385$ MHz, because the frequency of the line is $\nu = 115.271$ GHz.

The relevant values for the CO $J=1\rightarrow 0$ line are $g_1 = 1$, $g_2 = 3$, $A_{21} = 7.165 \cdot 10^{-8} \text{ s}^{-1}$ and $h\nu/k=5.53$ K.

5.1 Local Thermal Equilibrium

Let's first carry out the calculations for local thermal equilibrium. The optical depth

$$\tau_\nu = \int \alpha_\nu ds = \frac{h\nu}{4\pi} n_1 B_{12} (1 - e^{-\frac{h\nu}{kT}}) \phi_\nu(v) \Delta s$$

expressed in terms of A_{21} becomes

$$\tau_\nu = \frac{c^2}{8\pi\nu^2} n_1 \frac{g_2}{g_1} A_{21} (1 - e^{-\frac{h\nu}{kT}}) \phi_\nu(v) \Delta s.$$

We find $n_1 \Delta s = f_{n_1}(T) f_{\text{CO}} n \Delta s = f_{n_1}(T) \mathcal{N}_{\text{CO}}$ for thermal equilibrium by evaluating the Boltzmann distribution at 10 K. The relative occupation turns out to be $f_{n_1}(10) = 0.252$ (an easy way to check this can be carried out with RADEX by giving an extremely high density for the collision partner as input so that the levels become thermalised). This leads to $\tau_0 = 1.735$. As said before this is the optical depth of a square $\phi(\nu)$. It differs slightly from the centre of line optical depth of a Gaussian profile.

The radiative transfer equation in the Rayleigh–Jeans approximation becomes

$$T_R = T_{\text{bg}} e^{-\tau} + T(1 - e^{-\tau})$$

which yields 8.718 K for the total brightness at the frequency of interest. This corresponds to 5.983 K after beam switching against the background. But the Rayleigh–Jeans approximation is no longer valid at 115 GHz, so one does not get the correct Rayleigh–Jeans equivalent temperature this way either. Using the intensities, the beam-switched intensity becomes $2.234 \cdot 10^{-17} \text{ W m}^{-2} \text{ Hz}^{-1} \text{ ster}^{-1}$. This gives $T_B = 7.919$ K or $T_R = 5.472$ K.

5.2 Escape probability approximation

We now run this same problem through RADEX. The fractional occupation will now be larger for the lower level because the molecules will spontaneously decay more rapidly than collisions will repopulate the higher levels: $f_{n_1} = 0.4935$. This implies that the line is more optically thick, $\tau_0 = 2.345$. Furthermore the excitation temperature differs from the true temperature,

but this is a mild effect in this case: $T_{\text{ex}} = 8.403$ K. The resulting radiation temperatures are even lower: RADEX lists $T_B = 5.166$ K and $T_R = 4.610$ K.

Note that here the agreement is reasonably good. This is typical for CO, since the density of the cloud is close to the CO critical density, so the excitation is close to thermalisation. Also CO is simple and the background radiation is low, prohibiting complex excitation mechanisms. Furthermore, the line becomes optically thick, decreasing effectively the critical density.

The final worry is whether we will resolve this sphere and what we will measure as a result. Let's assume this source is at 1 kpc and we observe it with the IRAM 30m. We assume a beam of $21''$ and $\eta_A = 0.5$. Our source of 3000 AU only subtends $3''$. So even if the sphere has a uniform brightness (which is probably not correct, because it will be less optically thick towards the edges) the beam dilution is severe, $(3/21)^2 = 0.0204$. Thus, the observed antenna temperature is $0.0204 \times 4.610 \times 0.5 = 0.047$ K. With a single sideband system temperature of 150 K and a spectral line of width 0.385 MHz this requires 10 minutes on-source time to make a clear detection (with some assumption on correlator efficiency etc.). Another way of saying this is that the line flux density is almost 1 Jy.

Note that everybody makes a simplification in this last calculation by estimating the beam dilution against an empty sky. However the situation is in principle slightly more complex since the rest of the beam is filled with 2.73 K radiation, which does not add up on the position of our source, because it is opaque.

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