

MASA'S QUERIES

Moshe; April 18, 2017

Answers to Masa's queries from March 29, 2017. They should find their way to the MOLPOP-CEP manual.

1. At the end of the *.out file, I see `int(Tb dv) [K km/s]`.
Is this the value for molecular line flux at each J-transition?
I have used this value for my scientific interpretation.
Is this correct?

In the middle of this file, I also see `emission [erg/s/mol]`.
Is this also THE molecular line flux value at each J-transition?

I am confused about their relation. For reference, I attach
"HCN_LVGtest.inp" and "HCN_LVGtest.out". For simplicity,
IR pumping is not included in these files. For example,
for $N(\text{mol}) = 3.33\text{E}+12$,
J=1-0 : $6.09\text{E}-01$ [K km/s]
J=2-1 : $6.65\text{E}-01$ [K km/s]
J=3-2 : $1.95\text{E}-01$ [K km/s].

The J=2-1 to J=1-0 flux ratio is 1.09, and J=3-2 to J=1-0 flux ratio
is 0.32 in [K km/s].

On the other hand, if I use [erg/s/mol] in the middle, for $N(\text{mol}) = 3.33\text{E}+12$,
J=1-0 : $5.16\text{E}-21$ [erg/s/mol]
J=2-1 : $1.95\text{E}-20$ [erg/s/mol]
J=3-2 : $1.53\text{E}-20$ [erg/s/mol]

The J=2-1 to J=1-0 flux ratio is 3.78, and J=3-2 to J=1-0 flux ratio
is 2.97 in [erg/s/mol].

When we convert from [K km/s] to [erg/s], we need to multiply with
 ν^3 (ν is frequency). So when the J=2-1 to J=1-0 flux ratio in [K km/s]
is 1.09, the J=2-1 to J=1-0 flux ratio in [erg/s] should be $1.09 \times 8 = 8.72$.
When the J=3-2 to J=1-0 flux ratio in [K km/s] is 0.32, the J=3-2 to J=1-0
flux ratio in [erg/s] should be $0.32 \times 27 = 8.64$. However, the ratios in [erg/s]
in the *.out file are 3.78 and 2.97 for "J=2-1 to J=1-0" and "J=3-2 to J=1-0",
respectively, which are different from the above simple relation.
Could you please give me advice? Do I misunderstand anything?

Which of [K km/s] or [erg/s/mol] should I use for molecular line flux comparison with observations?

The quantity $\int T_b dv$ [K km/s] is calculated as follows: For uniform conditions, the line RJ-brightness temperature at frequency shift $x = v/\Delta v$ from line center, where Δv is the thermal linewidth, is found from

$$T_{br}(x) = T_{ex} \left(1 - e^{-\tau(x,\mu)}\right) \quad (1)$$

where T_{ex} is the line excitation temperature. The optical depth $\tau(x, \mu)$ is

$$\tau(x, \mu) = \frac{\tau_0}{\mu} e^{-x^2} \quad (2)$$

where τ_0 is the optical depth at line center and μ the viewing angle from the slab normal. Therefore, MOLPOP-CEP calculates the line-integrated brightness in K km s⁻¹ from

$$T_B \equiv \int T_{br} dv = T_{ex} \Delta v \int \left(1 - e^{-\tau(x)}\right) dx \quad (3)$$

In CEP runs, the integration is performed zone by zone, then added up.

The quantity emission [erg/s/mol] is calculated as follows: For a transition between upper level u and lower level l with frequency ν_{ul} , A -coefficient A_{ul} and escape probability β_{ul} , the emission in erg/s/mol is calculated from

$$ems(u, l) = h\nu_{ul} A_{ul} \beta_{ul} \frac{n_u}{n_{mol}} \quad (4)$$

where n_u is the number density of the upper level and n_{mol} is the molecular density. This quantity is the same as the line cooling factor j we introduced in Elitzur & Asensio Ramos 2006 (see eqs. 5 and 21 in that paper).

As you can see from the definitions, the quantities you consider are not related to each other with a simple multiplicative factor and you cannot infer their values for some transition from their values for another. Which one to use for comparison with observations depends very much on the data at hand and how it was obtained; that is why we list both, leaving the choice to the user.

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2. At the end of *.out file, I also see Flu [Jy] and Io [W/m/Hz/st].
I assume they are peak flux density. Since 1 [Jy] = 10^-26 [W/m/Hz],
these values are virtually identical except for "st". For example, for J=1-0,
N(mol) = 3.33E+12 : 5.82E+09 [Jy], 3.01E-18 [W/m/Hz/st]: ratio=0.52E-27
N(mol) = 5.93E+12 : 8.83E+09 [Jy], 4.86E-18 [W/m/Hz/st]: ratio=0.55E-27
N(mol) = 1.05E+13 : 1.28E+10 [Jy], 7.54E-18 [W/m/Hz/st]: ratio=0.59E-27
N(mol) = 3.33E+16 : 1.38E+11 [Jy], 1.10E-16 [W/m/Hz/st]: ratio=0.80E-27
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The ratios are different for different N(mol)? Why does this happen?
Is the solid angle different, depending on N(mol)? Namely, do you calculate the size of line emitting region and is it different depending on N(mol)?

I_0 is indeed the peak intensity but the line flux is actually the overall line emission explained above (the quantity *ems* in eq. 4) converted to Jy. We should indeed add all these definitions to the manual.

3. I used only LVG mode in MOLPOP, because I want to see the effect of IR pumping, when compared to RADEX calculations by collisional excitation. I refer to Elitzur & Asensio Ramos 2006 MNRAS 365 779.
Is this sufficient, since I use only LVG mode? May I write the webpage of MOLPOP?

Sure. If you want to compare to a RADEX LVG calculation you should use the LVG mode in MOLPOP.