In submillimetre astronomy, the observer usually obtains an antenna temperature, T_a , produced at a frequency ν by a source having an optical depth, τ :

$$au = rac{h}{\Lambda v} N_u B_{ul} (e^{h
u/kT} - 1)$$
 Equation 1

- N_u : column density of the upper state
- Δv: full width at half-maximum line width in units of velocity

 τ is computed by considering the probability that the emitted photon may escape from the relevant region, allowing for absorption at a rate $B_{ul} \rho$ where ρ is the energy density, and spontaneous emission at a rate A_{ul} along the path, and noting that:

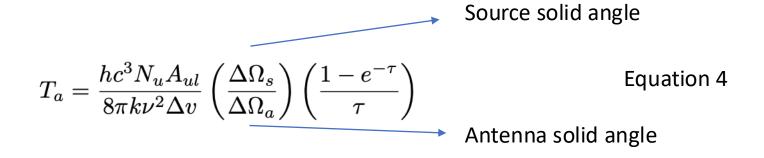
$$A_{ul}/B_{ul}=8\pi h \nu_{ul}^3/c^3$$
 Equation 2

[Recall that A_{ul} and B_{ul} are the Einstein coefficients for transitions between upper level u and lower level l]

We now need to introduce another concept, the brightness, B_{ν} (related of course to the brightness temperature), and relate it to the optical depth

$$\mathrm{B}_{
u} = rac{h
u/k}{e^{h
u/kT}-1} \left(rac{1-e^{- au}}{ au}
ight) au$$
 Equation 3

So that we can define the antenna temperature as:



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So that we can define the antenna temperature as:

$$T_a = \frac{hc^3N_uA_{ul}}{8\pi k\nu^2\Delta v} \left(\frac{\Delta\Omega_s}{\Delta\Omega_a}\right) \left(\frac{1-e^{-\tau}}{\tau}\right)$$
 Equation 4 Antenna solid angle

Note a very important concept: $T_a\Delta\nu$ is in fact the integrated line intensity over frequency (expressed in velocity here, and a measurable quantity):

$$W=\int T_a dv = T_a \Delta v$$
 Equation 5

In principle, N_u can be obtained by inverting Equation 4, in terms of the integrated line intensity to obtain:

$$N_u = \frac{8\pi k \nu^2 W}{hc^3 A_{ul}} \left(\frac{\Delta \Omega_a}{\Delta \Omega_s}\right) \left(\frac{\tau}{1-e^{-\tau}}\right)$$
 Equation 6

→ This is quite complex!

Often we can simplify this equation by making the following approximations (NOT ALWAYS VALID!):

- The source of emission (i.e the gas you are considering) fills the beam
- The emission of that particular line is optically thin

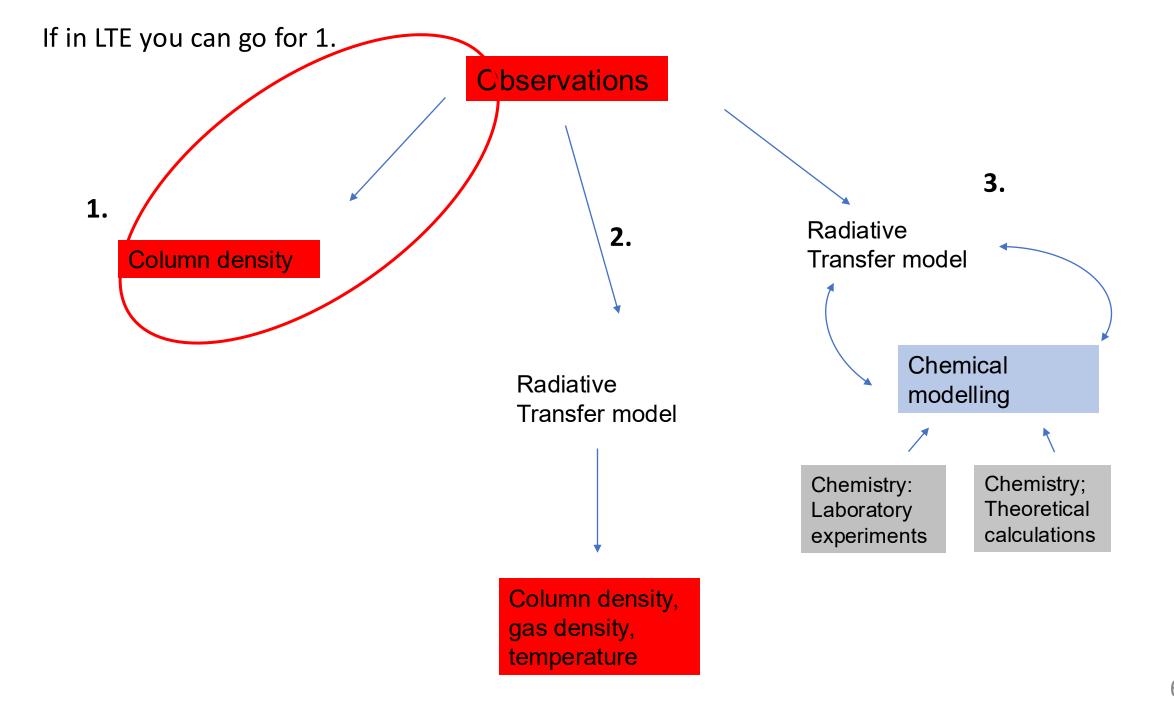
Can you see what happens if the above two statements are true?

$N_{\mu} \rightarrow N$

- In the previous lecture we provided and explained the meaning of the Antenna Temperature and its relationship with the column density of the upper state of the molecular transition observed.
- However, the actual quantity we want is the total column density of the observed species e.g. how much CO and hence H_2 is there in a galaxy? Or how much methanol can be produced in space?

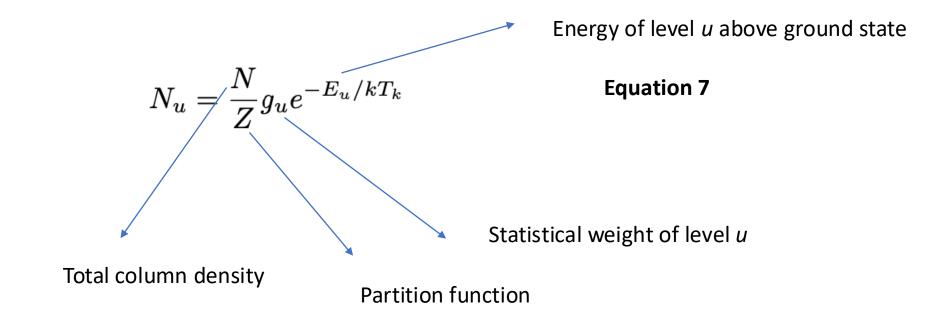
To derive this information, approximations must be made:

But first we need to know: Is the system in LTE? i.e do all the thermodynamical properties have thermodynamic equilibrium values at the *local* values of temperature and pressures?



LTE

• In LTE the total column densities of the observed species of the gas can be obtained from observation of a single transition



Now recall that:

$$N_{u} = \frac{8\pi k \nu^{2} W}{hc^{3} A_{ul}} \left(\frac{\Delta \Omega_{a}}{\Delta \Omega_{s}}\right) \left(\frac{\tau}{1 - e^{-\tau}}\right)$$

Equation 6

Or with the approximations we made (optically thin and emission arising from a region = beam size):

$$N_u = \frac{8\pi k \nu^2 W}{hc^3 A_{ul}}$$

We shall see a couple of practical examples shortly but first let's look a bit closer to this equation

$$N = \frac{Z}{g_u e^{\frac{-E_u}{kT_k}}} \frac{8\pi k v^2 W}{hc^3 A_{ul}}$$

Equation 8

Equation 8
$$N = \frac{Z}{g_u e^{\frac{-E_u}{kT_k}}} \frac{8\pi k v^2 W}{hc^3 A_{ul}}$$

We shall see a couple of practical examples shortly but first let's look a bit closer to this equation

 \boldsymbol{W} is the observation $\boldsymbol{\pi}$, k, h, c are constants

 $\mathbf{v}, \mathbf{g}_{uv} \mathbf{A}_{ulv} \mathbf{E}_{u}$ are functions of the molecular transition

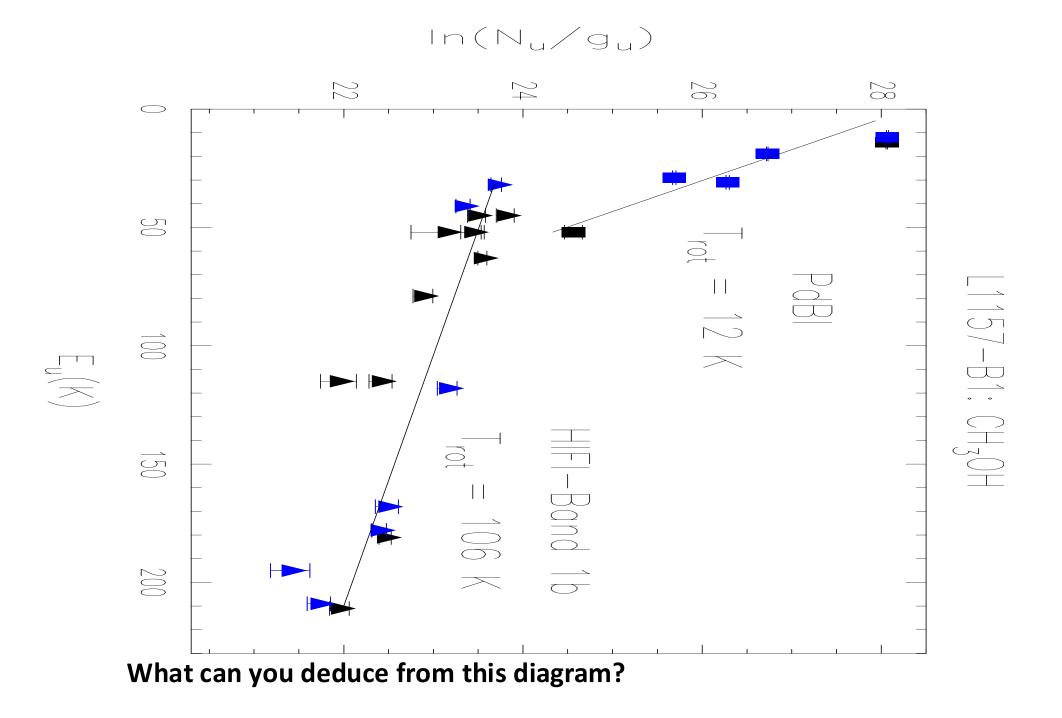
The partition function, Z, is a function of temperature T_k and while it can be calculated at different temperatures, for each molecule we often extrapolate it.

Clearly though there is still the real unknown which is the temperature (which ultimately is one the physical characteristics we want to derive from the observations!).

→ <u>Temperature can be deduced if more than one molecular transition of the same species</u> is observed

The rotational diagram

- From eq 7 you can construct a rotational diagram which relates the column density per statistical weight of a number of molecular energy levels to their energy above the ground state.
- The diagram is a plot of the natural logarithm of N_u/g_u versus E_u/k and, for Eq. 7, is a straight line with a negative slope of $1/T_k$
- The temperature inferred from such a diagram is often referred to as the rotational temperature and it is expected to be equal to the kinetic temperature if all the levels are thermalized.



Optical depth

The diagrams can also be used to assess whether the emission is optically thin or thick: if we rewrite Equation 7 as:

$$lnrac{N_u}{g_u} = lnN - lnZ - rac{E_u}{kT_k}$$
 Equation 9

we can include the possibility of finite optical depth by considering an optical correction factor $C_{\tau} = \tau/(1 - e^{-\tau})$ (from Equation 3 from previous lecture)

Close to unity in the optically thin case

$$lnrac{N_u^{thin}}{g_u} + lnC_{ au} = lnN - lnZ - rac{E_u}{kT_k}$$
 Equation 10

Summary so far:

- An optically thin transition produces an antenna temperature that is proportional to the column density in the upper level of the transition being observed
- If all the transitions are thermalized and we know the kinetic temperature, we can convert the single measured column density into the total column density of the species in question
- But if the emission is not optically thin the finite opacity produces an underestimate of the upper level column density of the observed transition as well as of the rotational temperature.
- The effects of optical depth are different depending on whether the molecule is linear or not.

However the observer is usually not aware whether the lines observed appear optically thin because the opacity is truly small or because the emission is beam diluted.

LTE: linear molecules – how to find the optical depth

$$\tau = \frac{h}{\Delta v} N_u B_{ul} (e^{h\nu/kT} - 1)$$

Rotational constant – NOT Einstein B coefficients!!

- Also recall that energy level = $E \sim BJ(J+1)$
- The statistical weight for linear molecules is $g_j = 2J + 1/2$
- Frequency of the transition $J \rightarrow J 1$ is given by $v_{J,J-1} = 2BJ$

 \rightarrow

$$A_{J,J-1} = \frac{64\pi^4 \nu^3 \mu^2}{3hc^3} \frac{J}{2J+1}$$

Equation 11

$$B_{J,J-1} = \frac{8\pi^3 \mu^2}{3h^2} \frac{J}{2J+1}$$

Equation 12

Using Equations 1, 7, 8, and 12, we can now then write the optical depth of this transition as:

$$\tau_{J,J-1} = \frac{8\pi^3 \mu^2}{3h} \frac{N}{\Delta v} \frac{1}{Z} J e^{-(B/kT)J(J+1)} (e^{2(B/kT)J} - 1)$$
 Equation 13

The variation of optical depth as a function of energy and J for a linear molecule in LTE is given by the above equation

If we are in a relatively warm cloud (not a prestellar core but e.g. a star forming region) then it can be shown that the partition function:

$$Z = kT/B$$

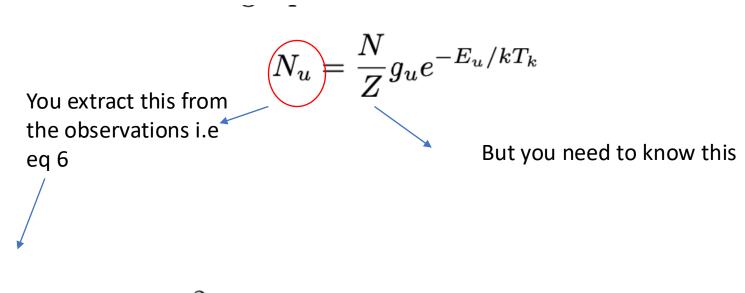
LTE: Nonlinear molecules

- For non linear molecules:
 - energy level structure quite complex
 - a complex dependence of transition frequencies on the energy upper state
 - a dependence on a larger range of H₂ densities for thermalization
 - a large range of absorption coefficients (i.e the optical depths vary considerably for a given molecular abundance).
- → Determining the optical depth has to be dealt with case by case.

For the "casual" submillimeter observer..be aware that

- Depending on the geometry of the emitting region as well as the transition and species observed, different formulae will apply
- The equation for the column density in one transition can be written in different formalisms depending:
 - on which transition is observed,
 - the type of region that is emitting it,
 - the spatial resolution of the instrument,
 - and whether all the relevant spectroscopic quantities for the transition are known.

$$N_u = rac{N}{Z} g_u e^{-E_u/kT_k}$$
 Equation 7



$$N_u = \frac{8\pi k \nu^2 W}{hc^3 A_{ul}}$$

The general recipe is to get: (1) expression for the partition function Z; (2) an expression for the total number density N

Let's look at one example of one molecule: N₂H⁺

N₂H⁺ (assuming optically thin)

This molecule is a linear rotor hence the partition function can be calculated by this formula:

$$Z_J = \sum_J (2J+1)exp\{-\frac{h}{kT}[B_0J(J+1)]\}$$

 $B_o = 46586.867 \text{ MHz}$

u

Let's assume you have observed the hyperfine transition 1-0 (recall equation 7):

 $N = \frac{8\pi W}{\lambda^3 A} \frac{g_l}{g_u} \frac{1}{T(R)_{ex} - T(R)_{bg}} \frac{1}{1 - exp(-h\nu/kT_{ex})}$

W = integrated intensity of the line

 $T(R)_{ex}$ and $T(R)_{bg}$ are the Rayleigh-Jeans excitation temperature and the temperature of a background source (i.e the cosmic microwave background radiation).

See paper by Goldsmith & Langer 1999 for other molecules e.g. CH₃OH

So far all the cases we have discussed were in LTE – but when does LTE apply?

- LTE applies when collision transition rates dominate over radiative transitions.
- However LTE is often never fully realized in the low densities of the interstellar medium.
- For any given transition, LTE is approached if the density exceeds a critical value, n_{crit} , , given by the ratio of the Einstein A-coefficient over the collisional rate (= A_{ii}/γ_{ii})
- From Equation 11 we saw that the A-coefficient scales as $\mu^2 v^3$
- However the decay rate is lowered by line trapping for optically thick lines so that the critical density is decreased.

Molecule	Formula	Transition	u GHz	E_u (K)	$n_{crit} \ (\mathrm{cm}^{-3})$	T(K)
Carbon Monoxide	CO	(1-0)	115.27	5.53	1.8×10^{3}	10
Carbon Monoxide	CO	(6-5)	691.47	116.16	$2.5{ imes}10^5$	100
Carbon Monosulfide	CS	(4-3)	195.95	23.51	$2.6{ imes}10^6$	20
Carbon Monosulfide	CS	(9-8)	440.80	105.79	$4.3{ imes}10^7$	100
Carbonyl Sulfide	ocs	(8-7)	97.30	21.01	$3.5{ imes}10^4$	20
Carbonyl Sulfide	ocs	(18-17)	218.90	99.81	$4.0{\times}10^5$	100
Sulfur Monoxide	\mathbf{SO}	(5_6-4_5)	219.95	34.98	$3.5{ imes}10^{6}$	50
Sulfur Monoxide	\mathbf{SO}	(8-8)	254.57	99.7	$2.8{ imes}10^{6}$	100
Sulfur Dioxide	SO_2	$(2_{20}$ - $2_{11})$	151.38	8.75	$8.7{ imes}10^{6}$	10
Sulfur Dioxide	SO_2	$(7_{44}-7_{35})$	357.39	69.47	$4.4{ imes}10^7$	75
Silicon Monoxide	SiO	(3-2)	130.27	12.50	$8.1{ imes}10^5$	10
Silicon Monoxide	SiO	(9-8)	390.73	93.77	$2.9{ imes}10^{7}$	100
Formyl Cation	HCO^{+}	(2-1)	178.38	12.84	$1.1{ imes}10^{6}$	10
Formyl Cation	HCO^{+}	(7-6)	624.21	119.84	$4.9{ imes}10^7$	100
Diazenylium	$\mathrm{N_2H^+}$	(2-1)	186.34	13.41	$9.2{ imes}10^5$	10
Diazenylium	$\mathrm{N_2H^+}$	(7-6)	652.09	125.19	$4.1{ imes}10^{7}$	100
Cyanoacetylene	$\mathrm{HC_{3}N}$	(12-11)	109.17	34.06	$7.1{ imes}10^5$	20
Cyanoacetylene	$\mathrm{HC_{3}N}$	(19-18)	172.85	82.96	$2.9{ imes}10^{6}$	80
Hydrogen Cyanide	HCN	(2-1)	177.26	12.76	1.0×10^{7}	10
Hydrogen Cyanide	HCN	(7-6)	620.30	119.09	$1.2{ imes}10^{9}$	100
Hydrogen Isocyanide	HNC	(3-2)	271.98	26.11	$8.0{ imes}10^{6}$	10
Hydrogen Isocyanide	HNC	(7-6)	543.89	91.37	7.6×10^{7}	100
Formaldehyde	$p-H_2CO$	$(2_{02}$ - $1_{10})$	145.60	10.48	1.1×10^{6}	10
Formaldehyde	$p-H_2CO$	$(3_{22}$ - $2_{21})$	218.47	68.00	$6.8{ imes}10^{6}$	70
Formaldehyde	$o-H_2CO$	$(2_{12}\text{-}1_{11})$	140.84	21.9	$8.8{ imes}10^{5}$	20
Formaldehyde	$o-H_2CO$	$(5_{15}$ - $4_{14})$	351.77	62.445	1.8×10^{7}	70
Methanol	e - CH_3OH	$(2_{00}$ - $1_{00})$	96.75	12.19	$2.8{ imes}10^{5}$	10
Methanol	e - CH_3OH	$(7_{30}$ - $6_{30})$	338.58	104.81	2.0×10^{7}	100
Methanol	a - CH_3OH	$(3_{00}$ – $2_{00})$	145.10	13.93	$1.8{ imes}10^{5}$	10
Methanol	a - CH_3OH	$(7_{-20}$ - $6_{-10})$	812.55	102.70	1.9×10^{8}	100
Deuterated Water	$^{\mathrm{HDO}}$	$(1_{01}$ - $0_{00})$	464.92	22.3	3.0×10^{6}	20
Deuterated Water	$^{\mathrm{HDO}}$	$(2_{11}$ - $2_{12})$	241.56	95.2	$1.1{ imes}10^{5}$	100
Isocyanic acid	HNCO	$(5_{05}-4_{04})$	109.90	15.8	1.0×10^{7}	20
Isocyanic acid	HNCO	$(15_{015}\text{-}14_{014})$	329.66	126.6	$1.2{\times}10^{8}$	80
Nitric Oxide	NO	$(3_{13} – 2_{-12})$	250.44	19.23	$2.4{ imes}10^{5}$	10
Nitric Oxide	NO	$(7_{18}-6_{-17})$	752.01	151.63	4.8×10^{7}	150

Examples of critical densities

- All we have discussed assumes a homogeneous emission region for each of the transitions observed.
- In reality, the ISM may be clumpy down to scales of hundredths of a parsec
- This means that while gas from within a beam of one transition may be in LTE, another transition of the same or a different species within the same beam may not be in LTE.

→ If the medium is homogeneous then it is relatively straightforward to determine whether the observed transition is in LTE; however, a truly homogeneous medium implies very small spatial scales.

- So, in reality, it is only when the emission is resolved and we can spatially disentangle the different gas components that we can be certain that LTE conditions apply.
- In most cases, and certainly for unresolved sources (especially distant galaxies) the beam will encompass a range of densities and temperatures, and LTE calculations will necessarily give only crude estimates of the densities and temperatures of the gas, and the column density of the species observed.
- Densities and temperatures derived from LTE calculations should always be treated as estimates rather than exact values.

The points above are key for a proper interpretation of what we observe in galaxies

Non-LTE

- If the medium is not thermalized, i.e, if the hydrogen density is not sufficient to thermalize some or all the transitions, a different temperature may characterize the population of each level relative to that of the ground state or relative to that of any other level.
- Recall that the excitation temperature T_{ex} , is defined by the relative populations or column densities of any two levels i and j of statistical weights gi and gj and energies Ei and Ej relative to an arbitrary common reference through the Boltzmann equation:

$$rac{N_j}{N_i} = rac{g_j}{g_i} e^{[-(E_j - E_i)/kT_{ex}]}$$
 Equation 14

- But if in non-LTE then a region of space can be affected by the radiation field and the total column density can no longer be obtained by using Equation 7
- Hence knowing the column density of one transition can not help you! → here you
 need to solve the radiative transfer equation (covered by other courses but see
 Further reading on Brightspace if you want to know more or see Chapter 9 in book)

From column densities \rightarrow to fractional abundances

- Often observers prefer to determine fractional abundances with respect to molecular hydrogen.
- In many cases, there is an advantage in obtaining fractional abundances: they are independent of geometry in that they give the total abundance (with respect to some form of hydrogen) of a species in the (assumed homogeneous) emitting region.
- There are several methods used by astronomers to convert molecular column densities to fractional abundances, depending on the optical thickness of the line(s) available, and on the extra information the observer has.

1. If one knows the column density of H_2 in the same emitting region \rightarrow

Then for species X its fractional abundance f(X) is simply:

$$f(x) = N(X)/N_{H2}$$

- 2. Or if not dust observations can provide us with measure of the optical depth of the region observed, and from there we derive the $\rm H_2$ column density by making the assumption (for the Milky Way) that in 1 magnitude of material we have $\sim 1.6 \times 10^{21}$ cm⁻² (in column density) of hydrogen nuclei.
- 3. But often beams from the dust observations differ from those of the molecular observations \rightarrow error associated with the H₂ density, and hence on the fractional abundance of the molecule

- 4. If no dust observations, we rely on CO observations: abundance of our molecule of interest can be derived as a fraction of CO
- \rightarrow then a standard CO/H₂ ratio is assumed.

Problems with this method:

- unless the beam size of the observations of the observed species and CO is the same, one suffers from beam dilution effects (as for method 3).
- The CO/H₂ ratio varies from galaxy to galaxy, as we shall see later in the course

Now, we move on to briefly describe how molecular observations can also provide much further insight into the physical conditions, and the history and dynamics of the gas if interpreted with the right tools.