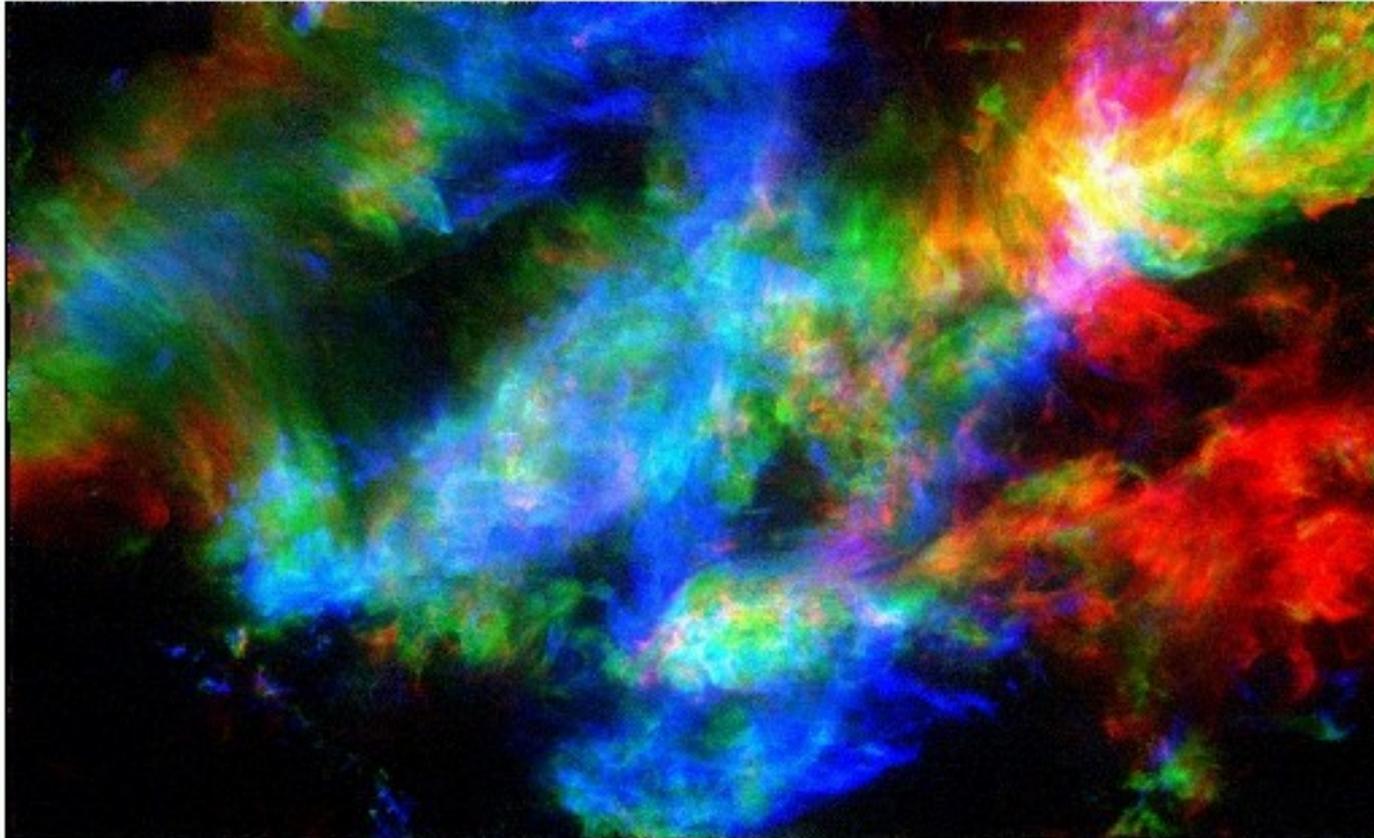


Molecules, mm & sub-mm (radio) astronomy



One of the last large projects completed with the **FCRAO 14-m telescope** was a map of 100 square degree region of the Taurus Molecular Cloud Complex in the emissions of the J=1-0 transitions of ^{12}CO and ^{13}CO . In addition to providing the distribution of molecular gas in this region, the high resolution spectra provide information on the cloud kinematics. The image below shows the ^{12}CO emission that is color coded, with red representing gas moving away, blue gas moving toward, and green gas moving at the average velocity of the cloud. **Ron Snell**

Molecules, mm & sub-mm (radio) astronomy

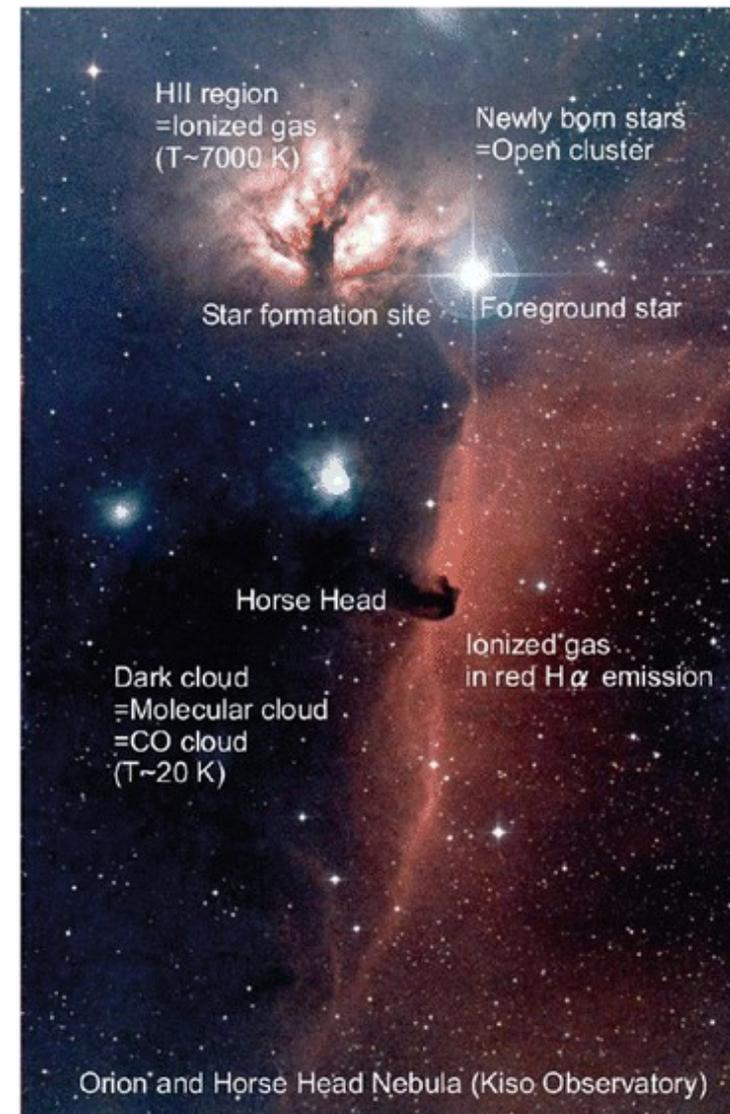
Further readings:

- Fanti & Fanti § 13.3 (only for generalities)
- Wilson, Rohlfs & Huttemeister "Tools of Radio Astronomy", chaps. 15-16
- Heyer & Dame "[Molecular Clouds in the Milky Way](#)"
2015, ARAA 53, 583-629 + a number of reviews cited at page 585
- Carilli & Walter "[Cool Gas in High Redshift Galaxies](#)"
2013, ARAA 51, 105-161

Molecules, mm & sub-mm (radio) astronomy

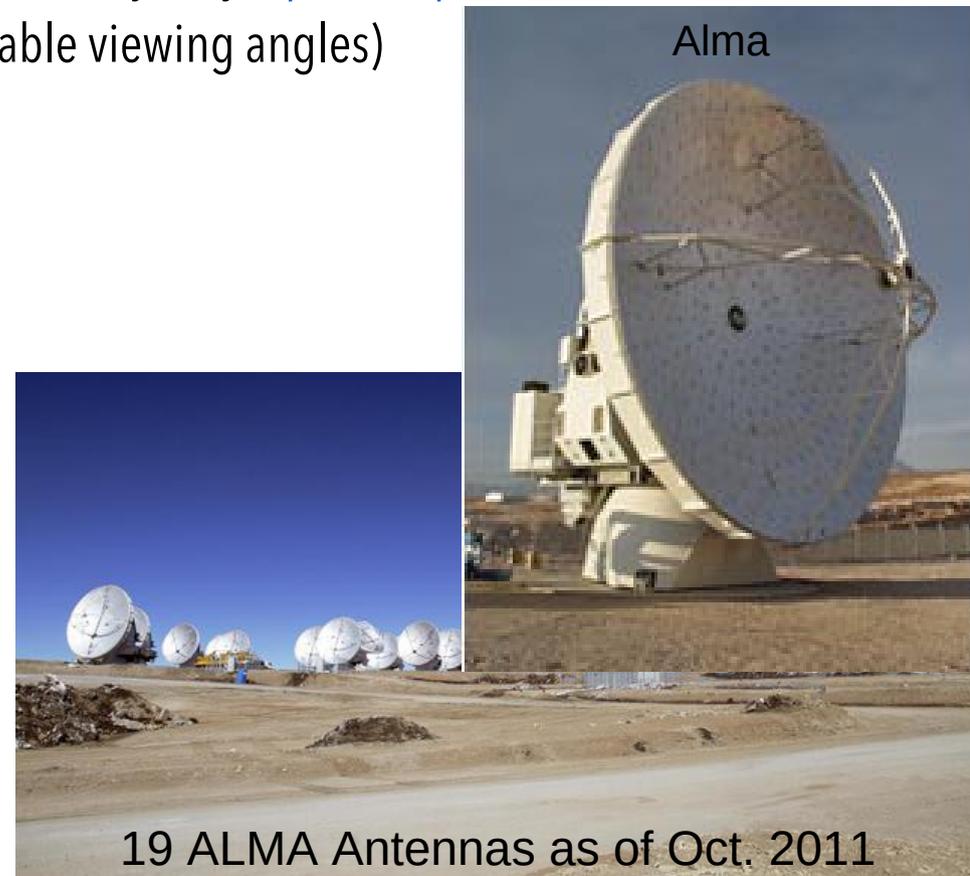
Existence of dense molecular clouds is one of the first clues to understand the formation of stars

- First visually identified as dark nebulae by William and Caroline Herschel (1785),
- Photographic observations of Barnard (1919) and Wolf (1923) established as discrete, optically opaque interstellar clouds.
- In **1950, discovery of the HI line** (21 cm emission): correlation between dust absorption and HI emission (Lilley, 1955). BUT, observations towards the centers of dark nebulae detected either very weak or no HI emission
- **Bok** et al. (1955) suggested that within these nebulae the gas had to be in molecular form.
- Cold molecular component of the interstellar medium (ISM) was discovered in **1970** (Wilson, Jefferts & Penzias, ApJL 161, 43-44) via **CO observations**. "We have detected intense line radiation from the direction of the Orion Nebula at a frequency of 115,271.2 MHz"



Molecules, mm & sub-mm (radio) astronomy

- Immediately realized that **dark clouds were made of molecules**, mainly consisting of molecular hydrogen mixed with small amounts of **interstellar dust** and trace amounts of more complex molecular species.
- **Molecular clouds are the sites of all star formation** in the Milky Way
- Our understanding of molecular clouds comes from the Milky Way (*optimal spatial resolution, bad distance evaluation*) and from external galaxies (favorable viewing angles)
- For about 40 years most studies conducted with moderate (~15m) to large (30-45m) telescopes plus a few interferometers made of a handful of antennas. Recently, ALMA provided resolution and sensitivity (collecting area!)

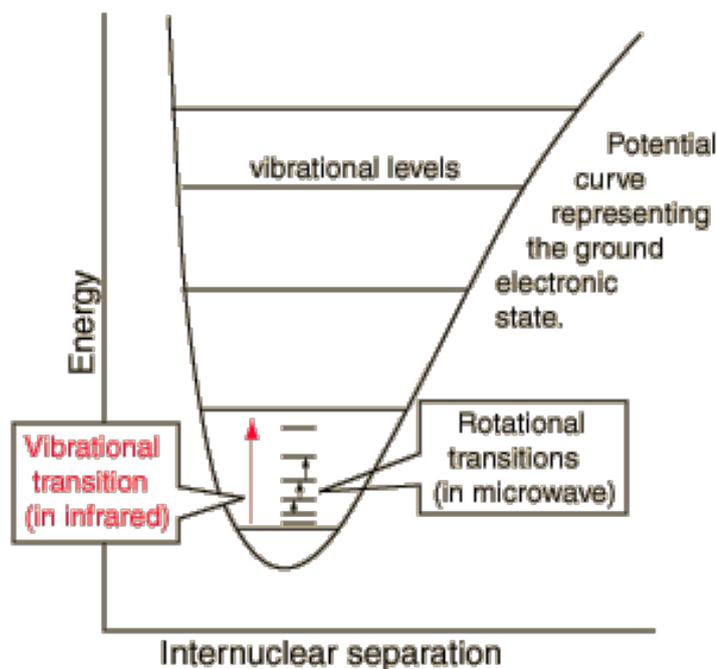
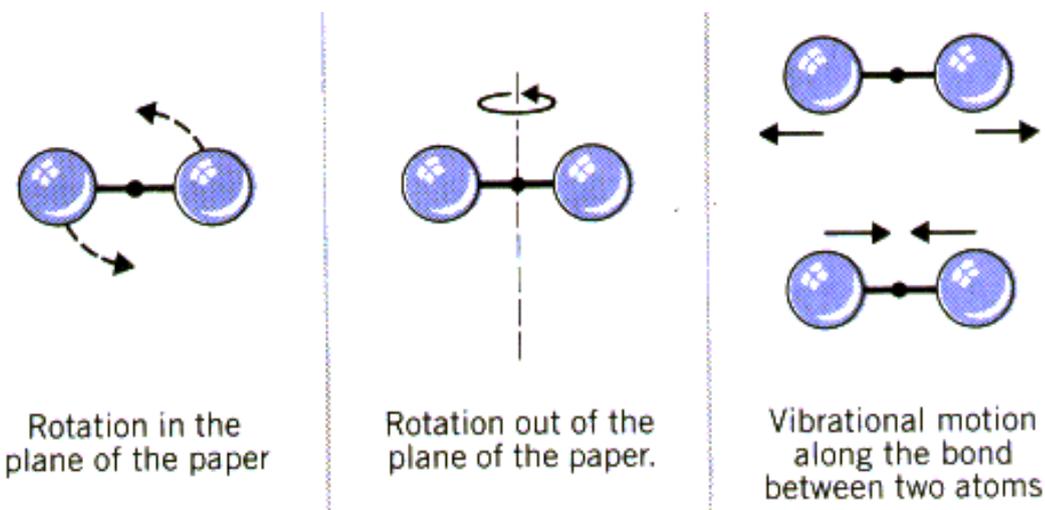


Molecules

Molecules are very difficult to deal with for quantum mechanics (positions and momenta of all components, nuclei & electrons, must be included in the Schrodinger equation)

Transitions grouped into 3 sets

- Electronic transitions ($\sim eV$)
- Vibrational transitions ($10 - 100 meV$)
- Rotational transitions ($\sim meV$)



(Born-Oppenheimer approximation)

Molecules: CO

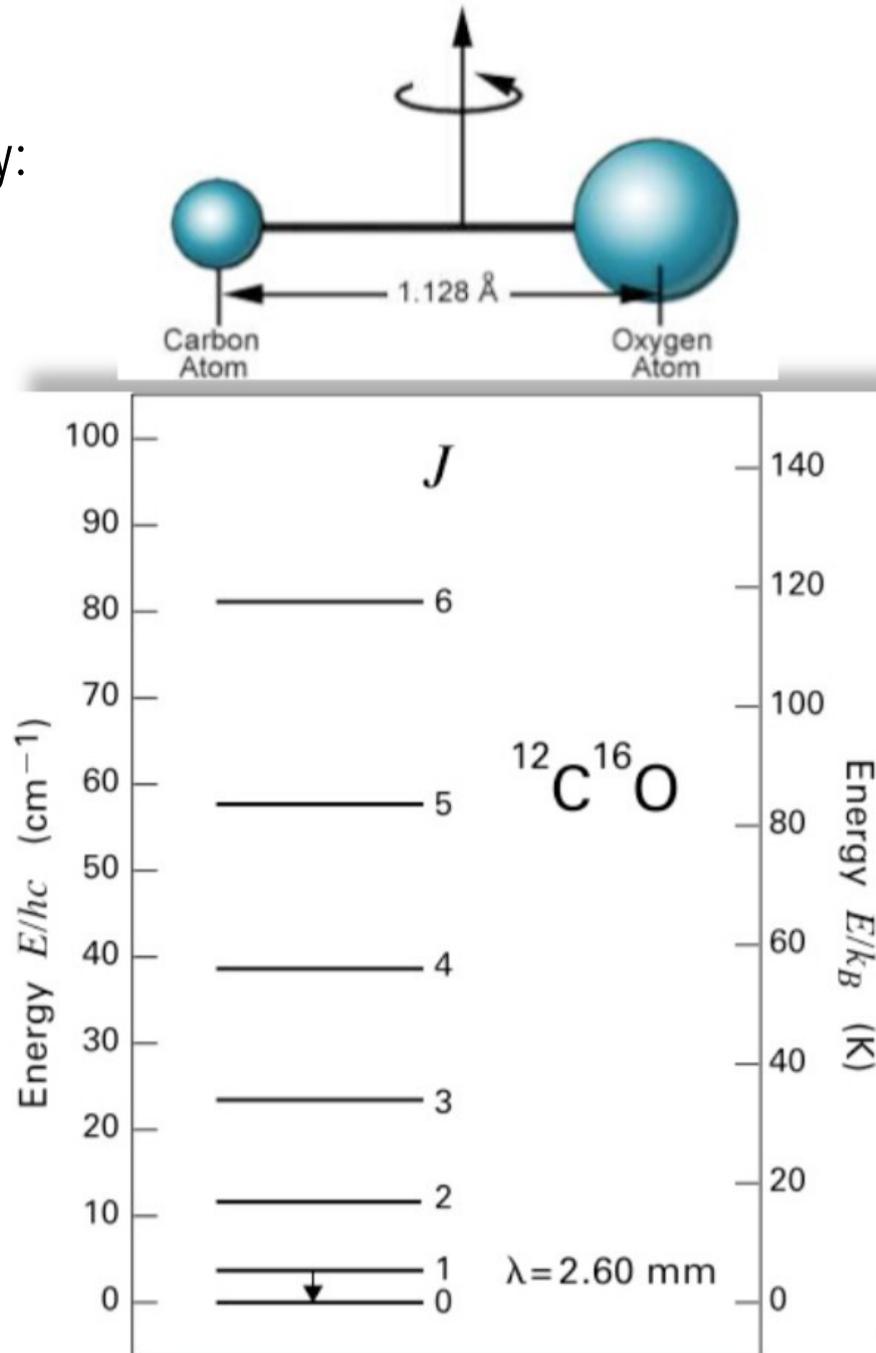
Quantum mechanics expression of the rotational energy:

$$E_{rot} = \frac{h}{2\pi I} J(J+1) \quad \text{with} \quad \Delta J = \pm 1$$

The $J=1$ state is elevated above the ground by $4.8 \cdot 10^{-4}$ eV or, equivalently, 5.5 K!

Easy to excite in a quiescent cloud.

Within a molecular cloud, excitation of CO to the $J=1$ level occurs primarily through collisions with the ambient H_2 .



Molecules with permanent dipole moments:

Aka: non – homonuclear

In the plane of rotation the dipole moment can be viewed as an antenna, oscillating as the molecule rotates.

Classically, the acceleration of positive and negative charges gives rise to radiation whose frequency is that of rotation frequency.

In the quantum mechanical model, the angular momentum is quantized, so that the radiation is emitted in discrete frequencies, when total angular momentum changes

Allowed dipole radiative transitions will occur between different rotational states only if the molecule is polar.

Homonuclear diatomic molecules (O_2 , H_2 , N_2) cannot undergo allowed transitions difficult to detect.

Molecular line measurement:

conversion of line intensity, integrated over linewidth, into column density.

$$M_{\text{CO}} = \text{Factor } D^2 \int_{\text{line}} I(\nu) d\nu \quad \text{units}$$

Aims:

1. Determine the complete chemical and isotopic content of a molecular cloud.
2. Relate the molecular clouds parameters to star formation
 - 2.1 Interaction with very young stellar objects
 - 2.2 Search for prebiotic molecules.

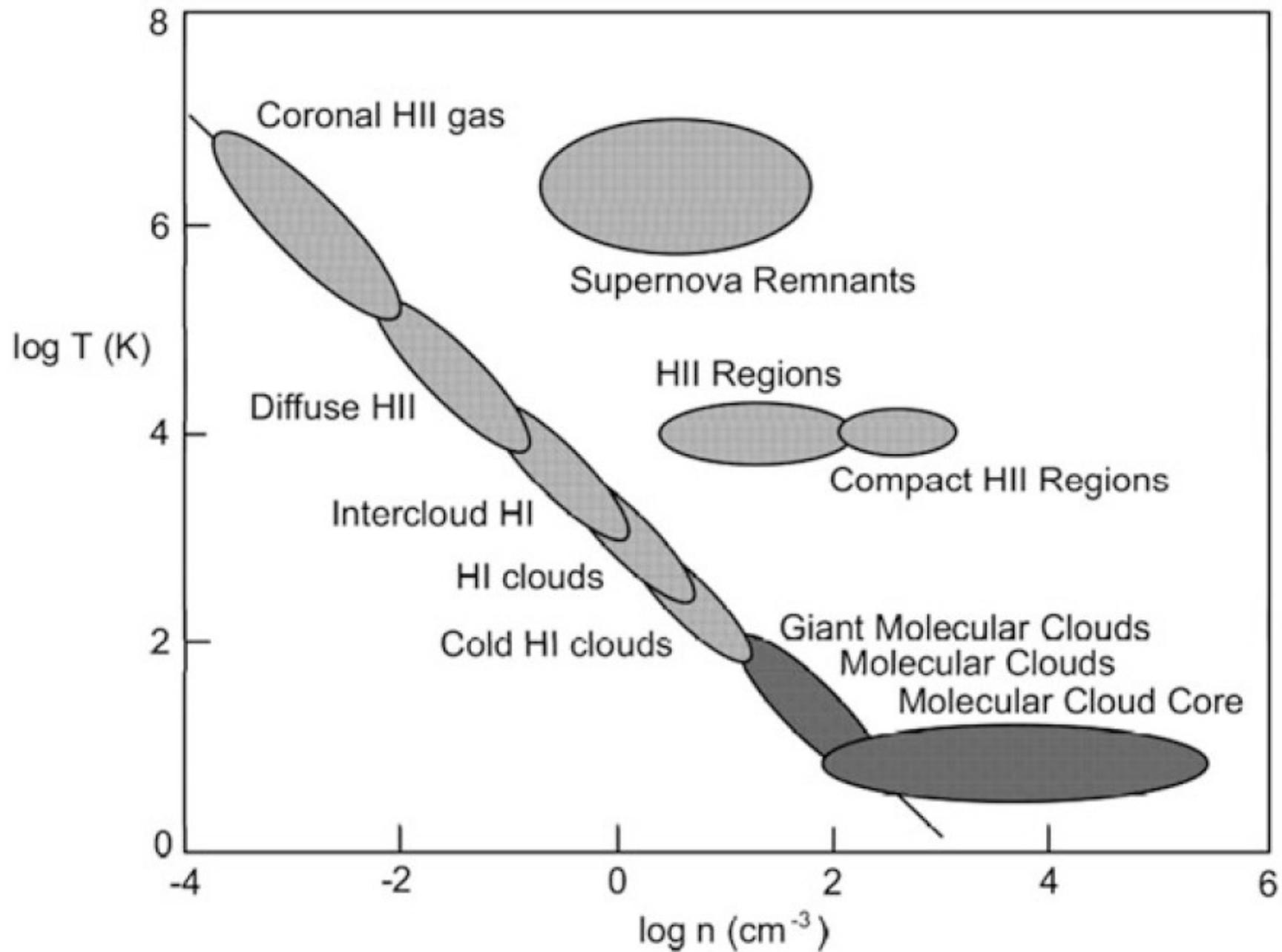


Table 2.1 ISM and radiations

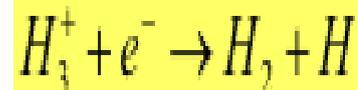
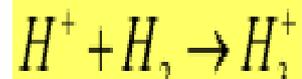
$T(K), E$	Object	Line	Continuum
2.7 K	CBR		mm,submm
10–50 K	Mol. cloud H ₂ gas Dust	Mol. lines mm,submm	FIR
100–1000 K	HI clouds Diffuse HI Dust	21-cm	IR
10 ⁴ K	HII regions	Recom.lines	Free-free
10 ^{5~7} K	SNR Diffuse HII Halo		Synch. X-rays
High-energy (keV-GeV)	Mag. fi, CR SNR, Pulsars Gal. Center AGN, Jets Radio gal.		Synch.Polari.
γ rays (GeV-TeV)	CR		γ rays

Molecule formation:

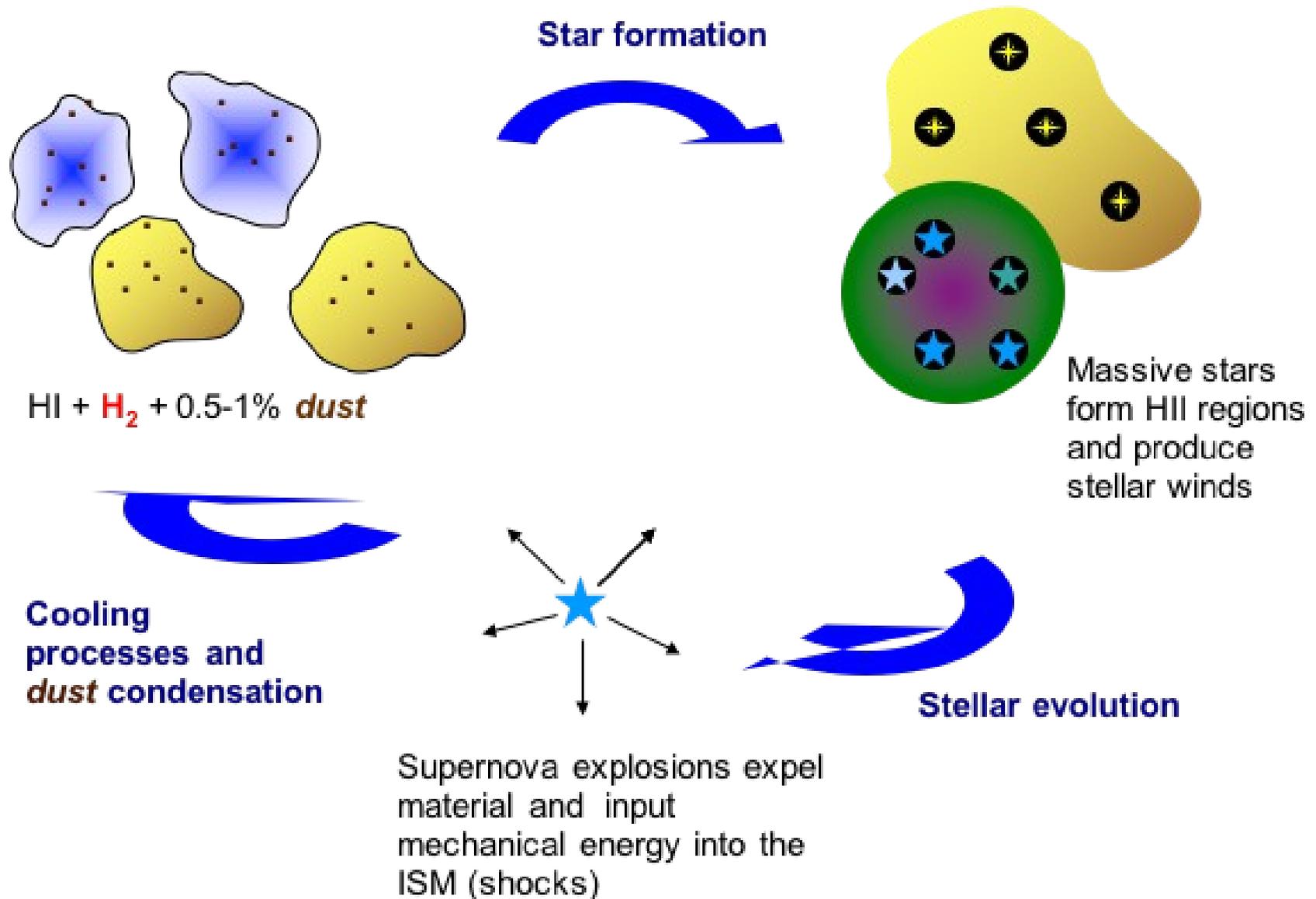
On dust grains, but a lot of details are unknown

Many possible reactions, but all are SLOW given LOW DENSITIES

Gas phase abundance of any species in a molecular cloud is a delicate balance between the production and destruction processes.



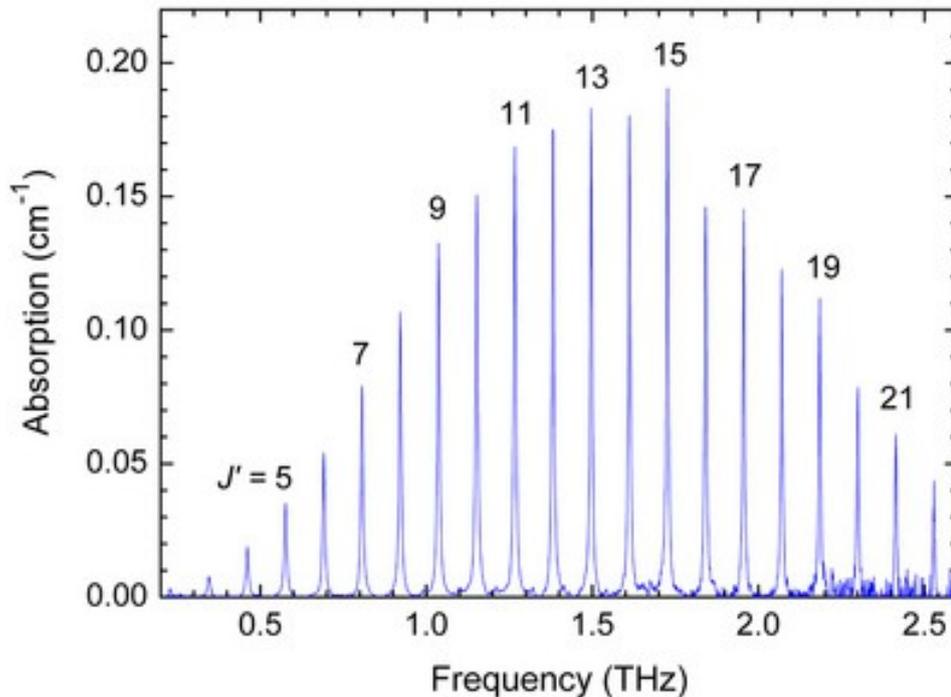
The interstellar medium energy cycle



- Stars form from dense, cool H_2
- The ISM plays an important role in the energy exchange and provides raw material
- Star formation occurs in dense dusty clouds so need some tracer that penetrates the dust ("extinction free" trace)
- Spectral observations also trace kinematics, so can be used to probe dynamical mass, gas motion, and gravitational torques
- Serves as fuel for both starburst and AGN activity
- Significant mass in galaxy nuclei
- H_2 is a "silent" molecule - need tracer species (CO)

Example of molecular transitions (model) for the CO

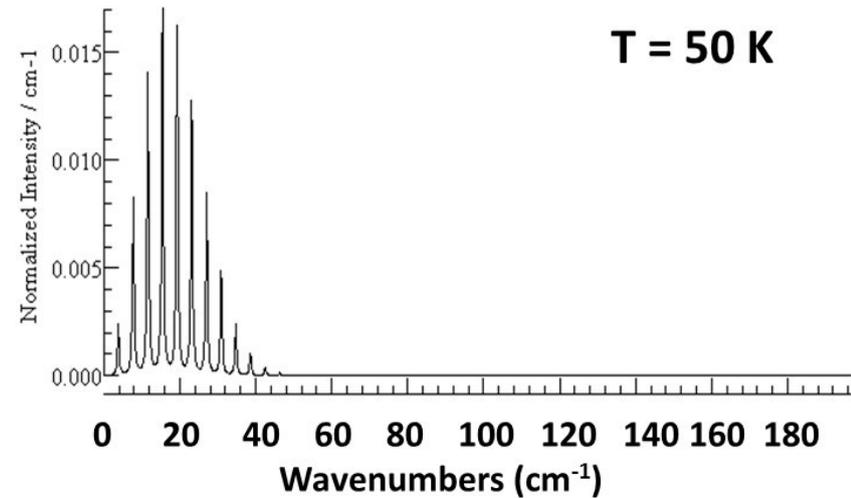
A rigid rotator is the model assumed



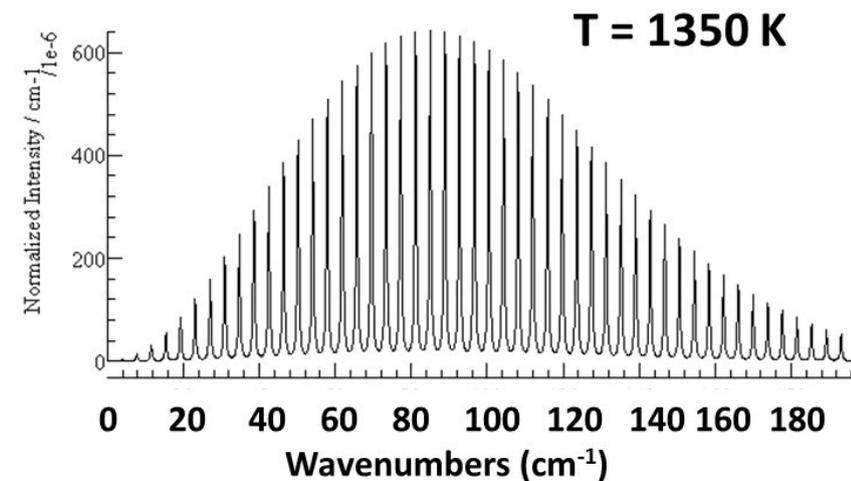
Laboratory CO spectrum in a 2 bar cell

CO Pure Rotational Spectrum

Temperature dependence due to the population of rotational energy levels.



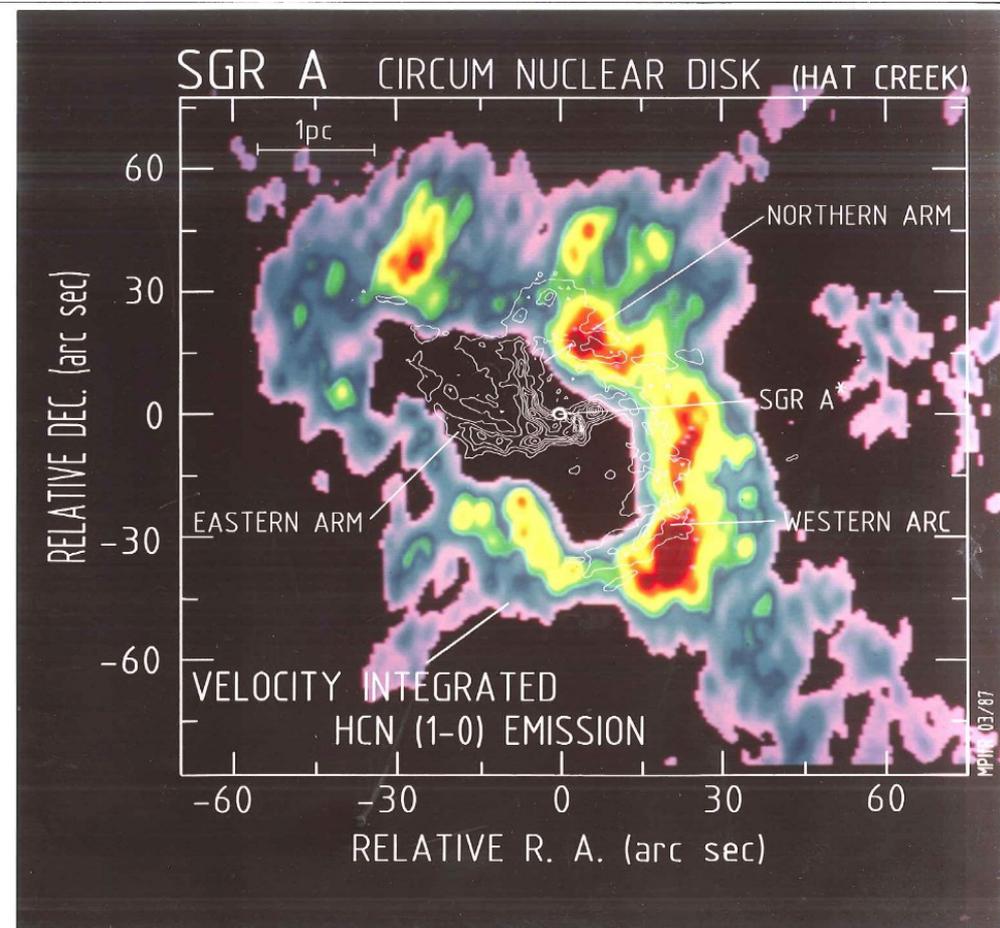
The maximum in J scales with kT .



Complex molecules (3+ elements) have more and more complicated energy levels, depending on geometry. There is coupling with the electric dipole/quadrupole and magnetic dipole of the e- and nuclei and all this produces hyperfine transitions, splitting single levels in multiple line profiles with tiny separation in energy.

The energy separation (as small as a few MHz) depends on the position of a given nucleus in the molecule.

e.g. HCN and HNC have different level separation



All dipole transitions are allowed and will occur only in case the molecule is polar

Homonuclear molecules (O_2 , H_2 , N_2 , C_2 , ...) difficult to detect and have forbidden transitions:

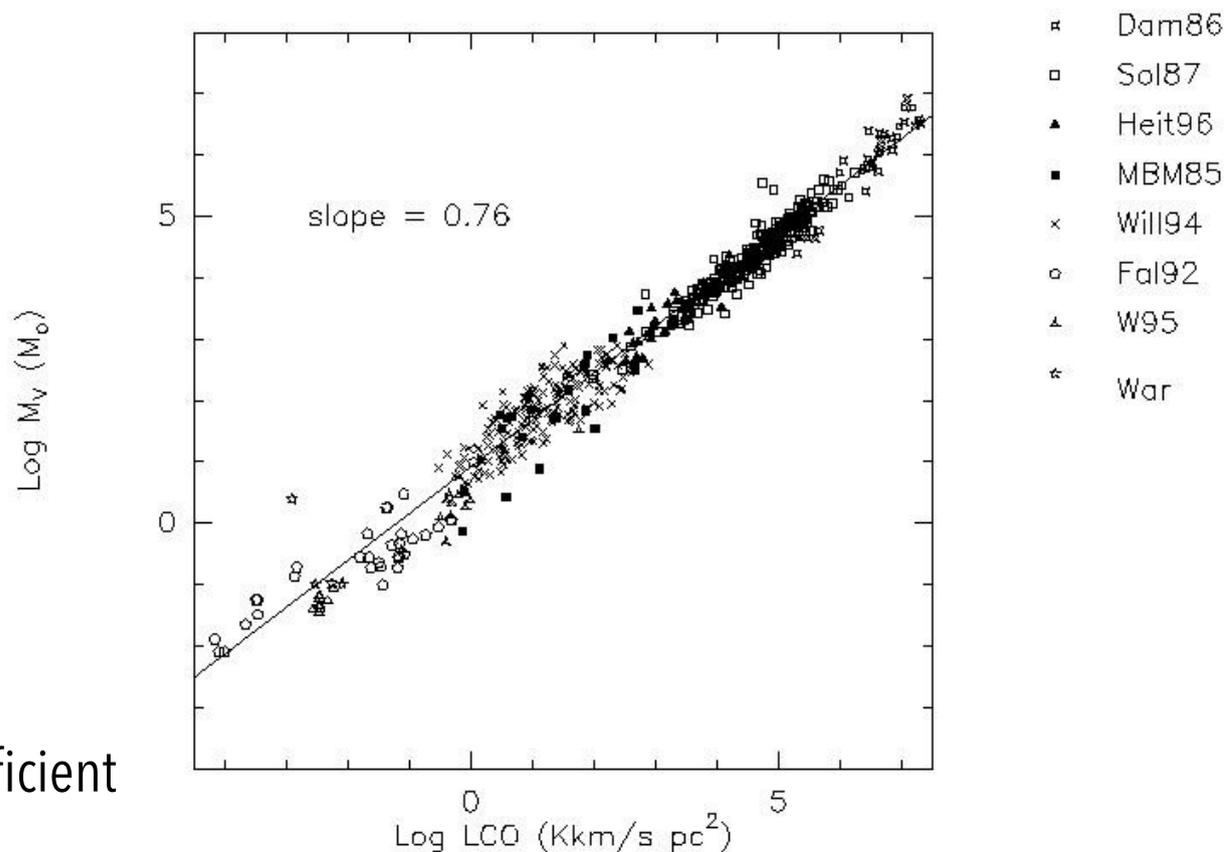
H_2 has large spacings of the rotational levels: first quadrupole line ~ 500 K above ground level (inefficient radiation from most of the cold ISM (where $T < 200$ K)

Detected/evaluated via tracers

- Extinction + thermal continuum emission from dust grains
- Gamma rays from CR collisions
- Molecular line spectroscopy (^{12}CO , ^{13}CO , $C^{18}O$)

CO has a small dipole moment and a correspondingly small Einstein A coefficient

CO is the best tracer of H_2



Virial mass .vs. CO luminosity

Critical density:
$$\frac{A_{ul}}{n_p Q_{ul}} = 1 \quad \rightarrow \quad \text{namely} \quad \rightarrow \quad n_p^{cr} = \frac{A_{ul}}{Q_{ul}}$$

It is different for each transition! CO J1 → 0, has a critical density of ~ 2000 cm⁻³.

Dense regions ensure a consistent population of the excited state (kinetic temperature)

CO forms in regions where visual extinction is > 1-3 Mag, dense enough that the line is optically thick: i.e. Emitted photons absorbed by another molecule

¹²CO complemented with ¹³CO (25-100 less abundant)

moderate optical depth, and then more appropriate to determine H₂ in dense regions

CO and H₂ are linked since formed and destroyed by similar physical processes:

Formation: surface of dust grains

Dissociation: H₂

- 1. incident UV photon excite molecule to Lyman ($\lambda < 1108 \text{ \AA}$) or Werner ($\lambda < 1008 \text{ \AA}$) bands*
- 2. ~15% radiative de excitation into unbound within the electronic ground level that dissociated the molecule*

Penetration of UV photons limited by dust attenuation + opacity provided by the outer H₂ layer ($\tau \sim \mu l$, then deeper in the cloud higher τ , all H₂ molecular)

Competition between radiative and collisional de-excitation quantified by ratio C_{ul}/A_{ul}

Critical density n_{crit} for which

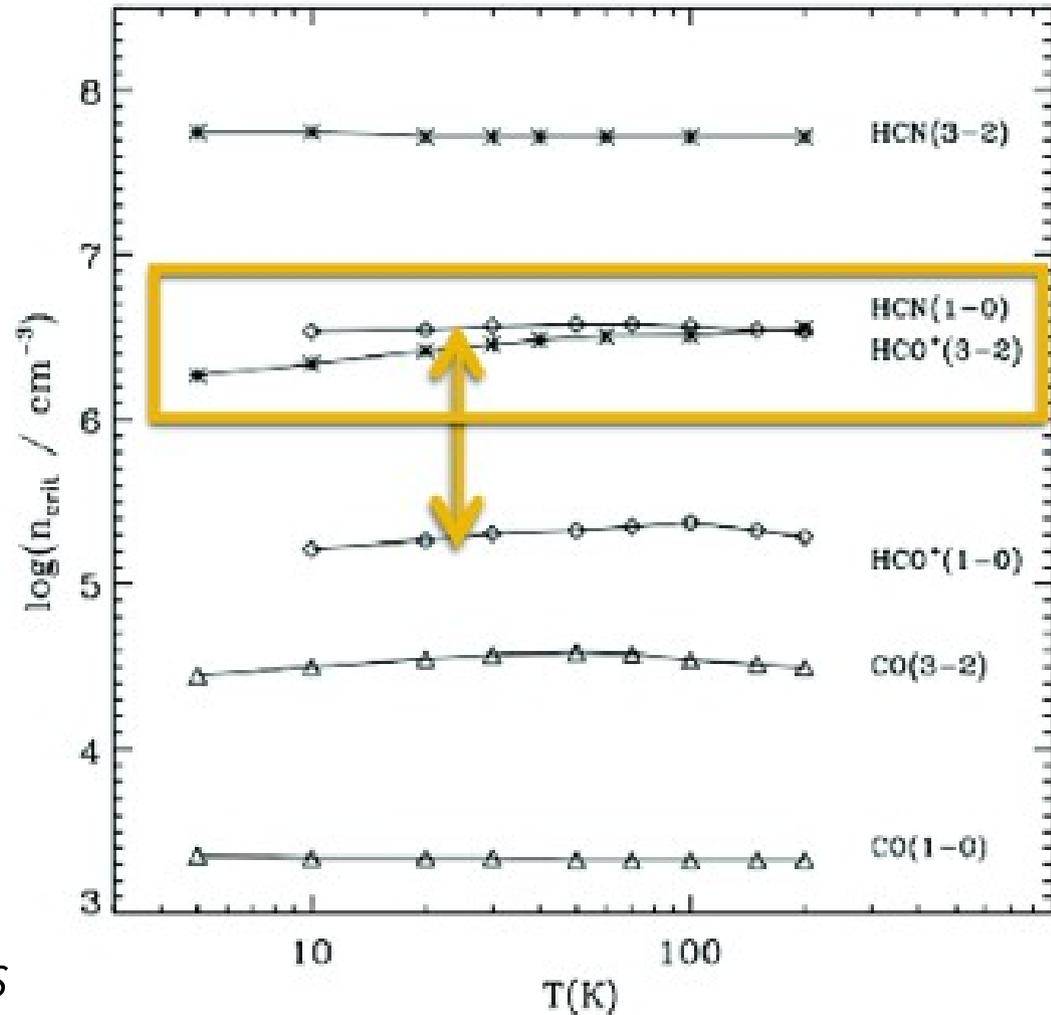
$$A_{ul}/C_{ul} = 1 \sim J^3 m_{el}^2 / n(H_2) T^{1/2}$$

m_{el} = electric dipole moment,

J = angular momentum quantum number

Highest n_{crit} molecules with largest m_{el} trace **hottest/densest** molecular gas.

On the same molecule, highest-order transitions trace **hottest/densest** molecular gas



CO emission is optically thick (e.g., Wilson+ 1974), hence traces surface area

Not suitable for estimating total gas amount. Need optically thin emission (all photons detected)

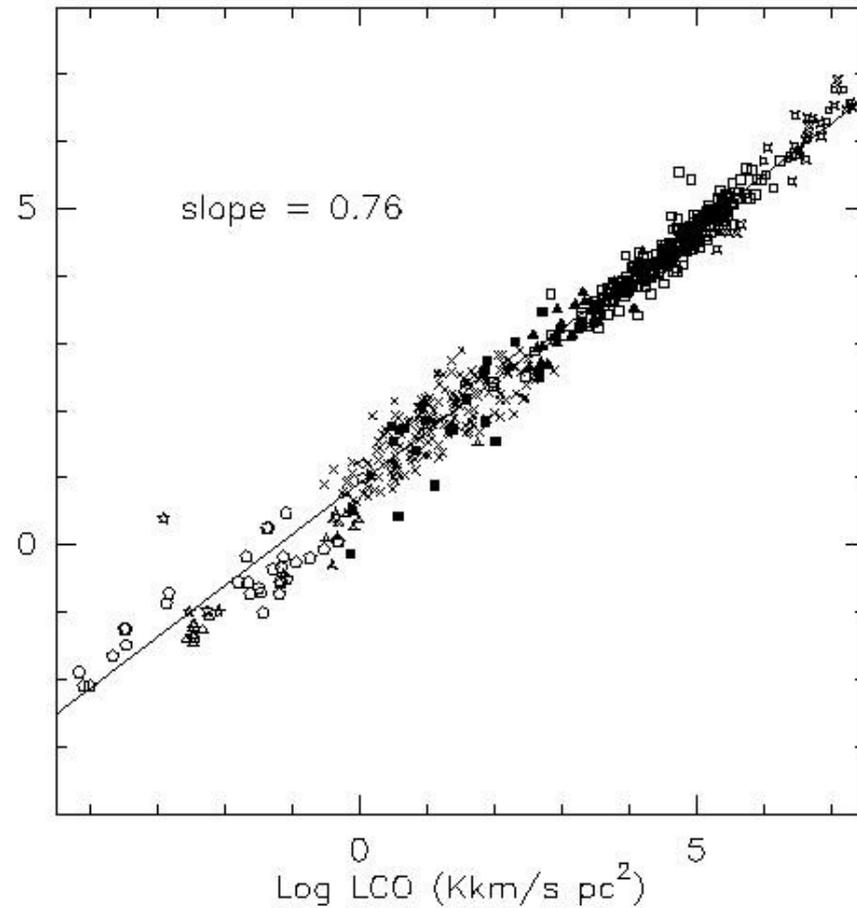
Critical density & temperature

Species	Transition	Excitation potential (K)	λ (Å)	ν (GHz)	Einstein A (s^{-1})	n_{crit} (cm^{-3})
CO	J = 1-0	5.5	2601	115.27	7.2×10^{-8}	2.1×10^3
	J = 2-1	16.6	1300	230.54	6.9×10^{-7}	1.1×10^4
	J = 3-2	33.2	867	345.80	2.5×10^{-6}	3.6×10^4
	J = 4-3	55.3	650.3	461.04	6.1×10^{-6}	8.7×10^4
	J = 5-4	83.0	520.2	576.27	1.2×10^{-5}	1.7×10^5
	J = 6-5	116.2	433.6	691.47	2.1×10^{-5}	2.9×10^5
	J = 7-6	154.9	371.7	806.65	3.4×10^{-5}	4.5×10^5
	J = 8-7	199.1	325.2	921.80	5.1×10^{-5}	6.4×10^5
	J = 9-8	248.9	289.1	1036.9	7.3×10^{-5}	8.7×10^5
	J = 10-9	304.2	260.2	1152.0	1.0×10^{-4}	1.1×10^6
HCN	J = 1-0	4.25	3383	88.63	2.4×10^{-5}	2.6×10^6
	J = 2-1	12.76	1691	177.26	2.3×10^{-4}	1.8×10^7
	J = 3-2	25.52	1128	265.89	8.4×10^{-4}	6.8×10^7
	J = 4-3	42.53	845.7	354.51	2.1×10^{-3}	1.8×10^8
	J = 5-4	63.80	676.5	443.12	4.1×10^{-3}	3.8×10^8
	J = 6-5	89.32	563.8	531.72	7.2×10^{-3}	7.1×10^8
	J = 7-6	119.09	483.3	620.30	1.2×10^{-2}	1.2×10^9

Detected/evaluated via tracers

- Extinction + thermal continuum emission from dust grains
- Gamma rays from CR collisions
- Molecular line spectroscopy (^{12}CO , ^{13}CO , C^{18}O)

Log $M_V (M_\odot)$



Virial mass .vs. CO luminosity

How to find the H_2 abundance: the X_{CO} factor:

$$X_{\text{CO}} = 1.6 \cdot 10^{19} \frac{T_{\text{ex}}}{30\text{K}} e^{\frac{5.5\text{K}}{T_{\text{ex}}} - 0.184} \text{cm}^{-2} (\text{K km s}^{-1})^{-1}$$

Method	$X_{\text{CO}} / 10^{20}$ $\text{cm}^{-2}(\text{K km s}^{-1})^{-1}$	References
Virial	2.1	Solomon et al. (1987)
	2.8	Scoville et al. (1987)
Isotopologues	1.8	Goldsmith et al. (2008)
Extinction	1.8	Frerking, Langer & Wilson (1982)
	2.9-4.2	Lombardi, Alves & Lada (2006)
	0.9-3.0	Pineda, Caselli & Goodman (2008)
	2.1	Pineda et al. (2010)
	1.7-2.3	Paradis et al. (2012)
Dust Emission	1.8	Dame, Hartmann & Thaddeus (2001)
	2.5	Planck Collaboration et al. (2011a)
γ -rays	1.9	Strong & Mattox (1996)
	1.7	Grenier, Casandjian & Terrier (2005)
	0.9-1.9 *	Abdo et al. (2010d)
	1.9-2.1 *	Ackermann et al. (2011, 2012d)
	0.7-1.0 *	Ackermann et al. (2012b, 2012c)

H_2 column density

$$N_{\text{H}_2} = X_{\text{CO}} W_{\text{CO}} = X_{\text{CO}} \left(\int T_{\text{B}}(v) dv \text{ K km s}^{-1} \right) \text{ cm}^{-2}$$

Fact:

⇒ Stars form in high density regions

High-density molecular tracers: HCN(1-0)

Correlation:

IR luminosity (\sim SFR) and

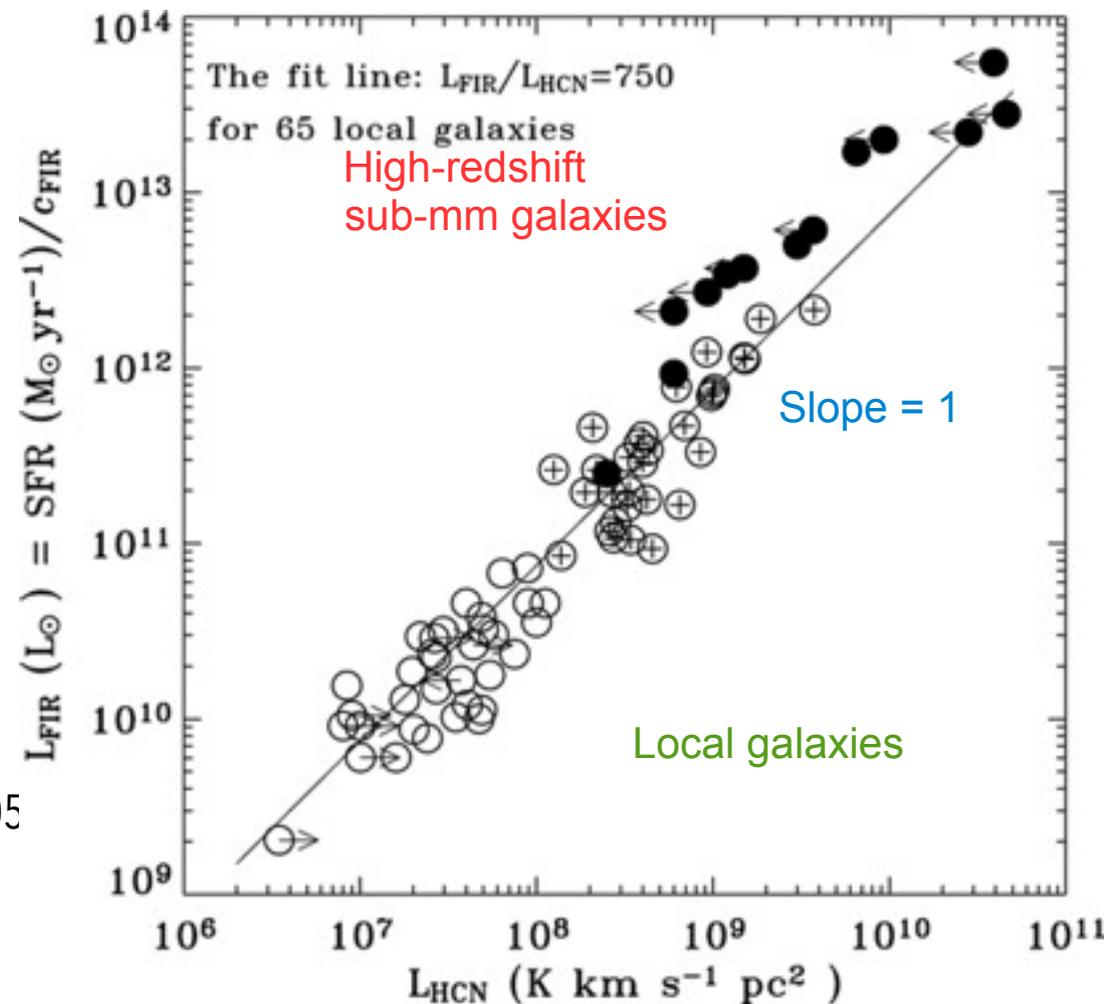
HCN J=1-0 luminosity

(\sim mass of gas above critical density)

(Gao & Solomon 2004, Gao+ 2007, see also Wu+ 2005)

Linear (rather than super-linear as for CO);

dense gas more closely correlated with star formation.



Fact:

$$A_{ul}/C_{ul} = 1 \sim J^3 m_{el}^2 / n(H_2) T^{1/2}$$

Einstein A_{ul} coefficient $\sim J^3 m_{el}^2$

i.e. : dense regions are transparent to high m_{el}^2 & high J transitions

➡ Best dense gas tracers :

CS ($m_{el} = 1.958$ Debye),

HCO⁺ ($m_{el} = 3.93$ Debye)

HCN ($m_{el} = 2.985$ Debye)

NH₃ ($m_{el} = 1.48$ Debye)

CO ($m_{el} = 0.110$ Debye) is less favorable, and it is a good tracer of moderately dense regions

➡ Which molecule is more convenient is determined by relative abundances (and observational requirements as well!)

Which molecule is more convenient is determined by relative abundances
(and observational requirements as well!)

CS (Carbon Monosulfide)

transitions in (J1-0 @ 48.99 GHz) mm & submm bands, level separation a few tens of GHz

HCO⁺ ()

HCN (Hydrogen Cyanide)

transitions in (J1-0 @ 88.63 GHz) mm & submm bands, level separation a few tens of GHz

HNC (Hydrogen Isocyanide)

transitions in (J1-0 @ 90.66 GHz) mm & submm bands, level separation a few tens of GHz

NH₃ (para & ortho ammonia)

transitions in radio (many between 23 & 25 GHz, wide range of temperatures) excellent to study protostellar cores !

Parameters for transitions of the most common interstellar molecules in table 16.1, Tool of Radio Astronomy

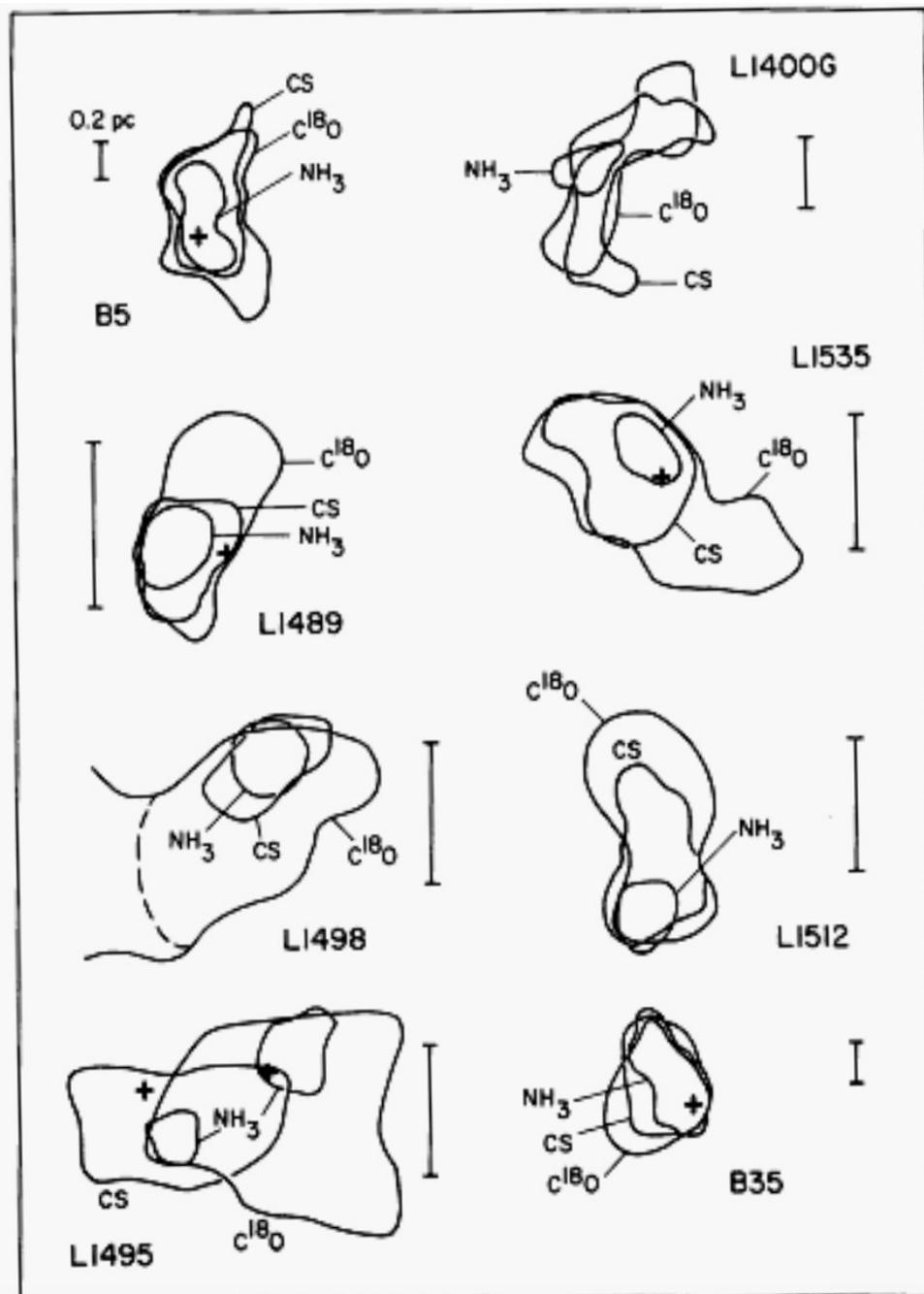


FIG. 1a

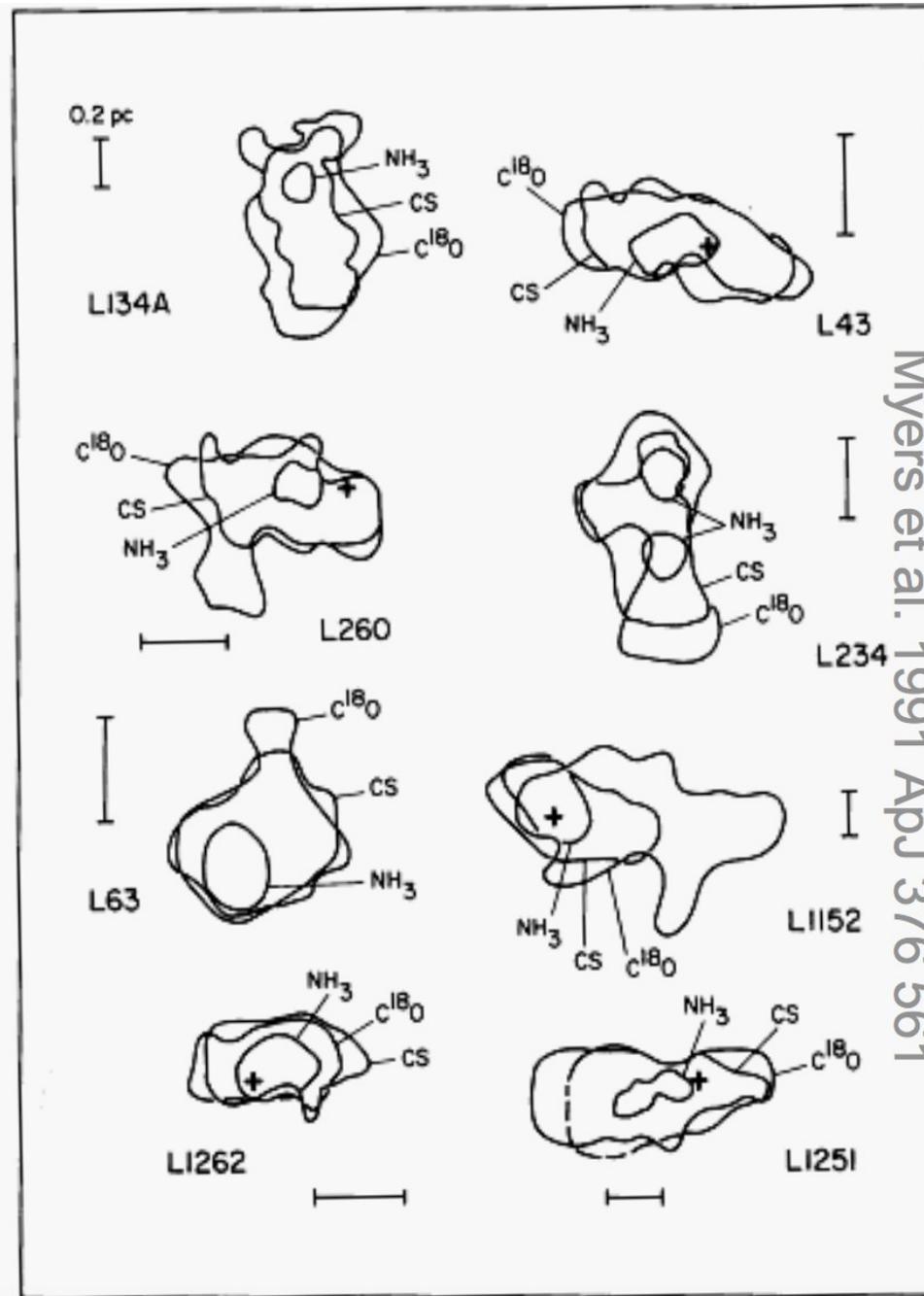


FIG. 1b

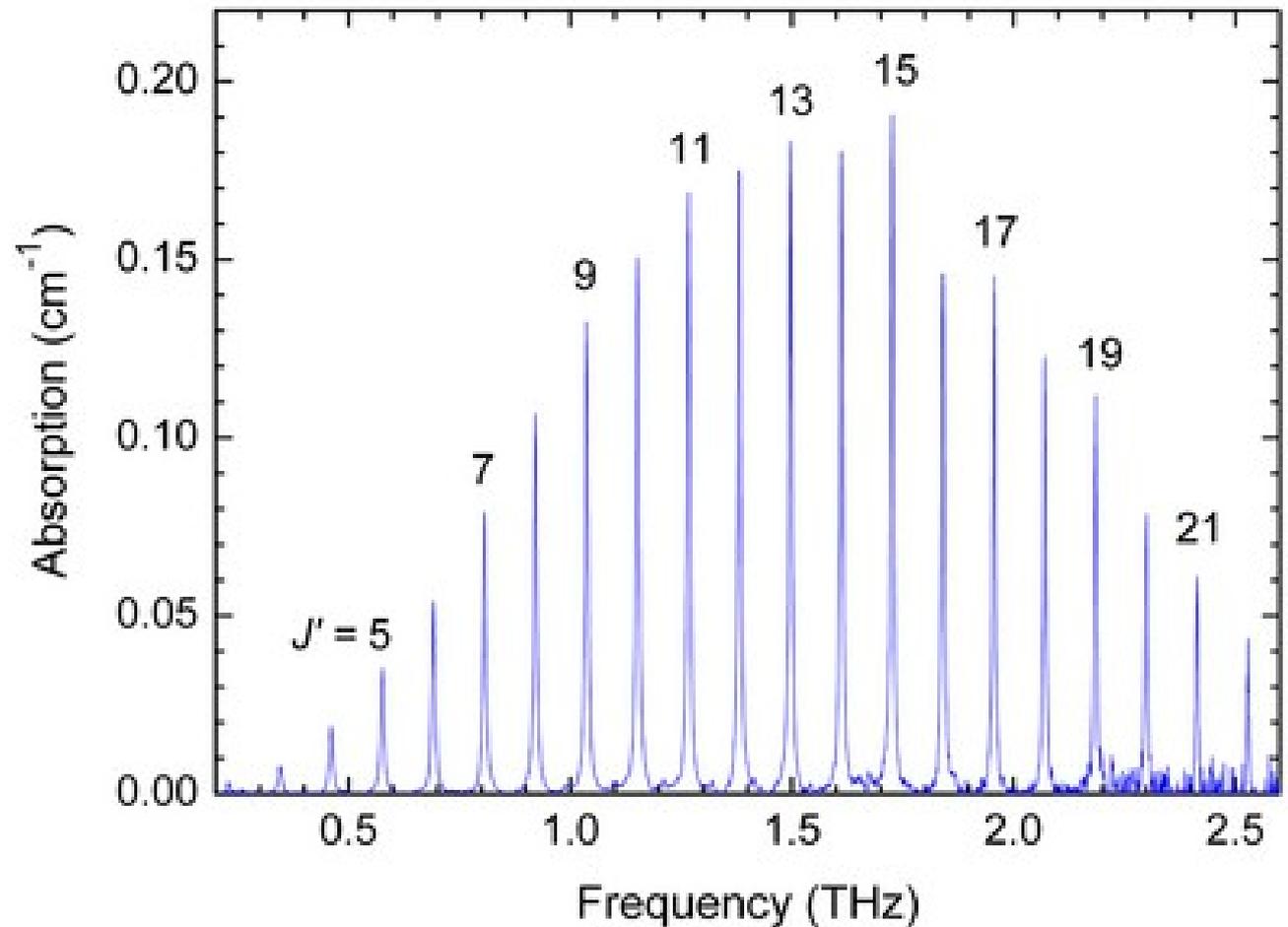
Brightness temperature related to the temperature of τ_{CO} surface

Firstly detect at least three lines (more is better!)

Line ratios determine T_{ex} (which should be the same if Emission is optically thin)

X_{CO} factor here better written

Terahertz transmission spectrum of a CO cell at 2 bar pressure



How to find the H_2 abundance: the X_{CO} factor:

$$X_{CO} = 1.6 \cdot 10^{19} \frac{T_{ex}}{30K} e^{\frac{5.5K}{T_{ex}} - 0.184} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1}$$

A black hole mass measurement from molecular gas kinematics in NGC4526

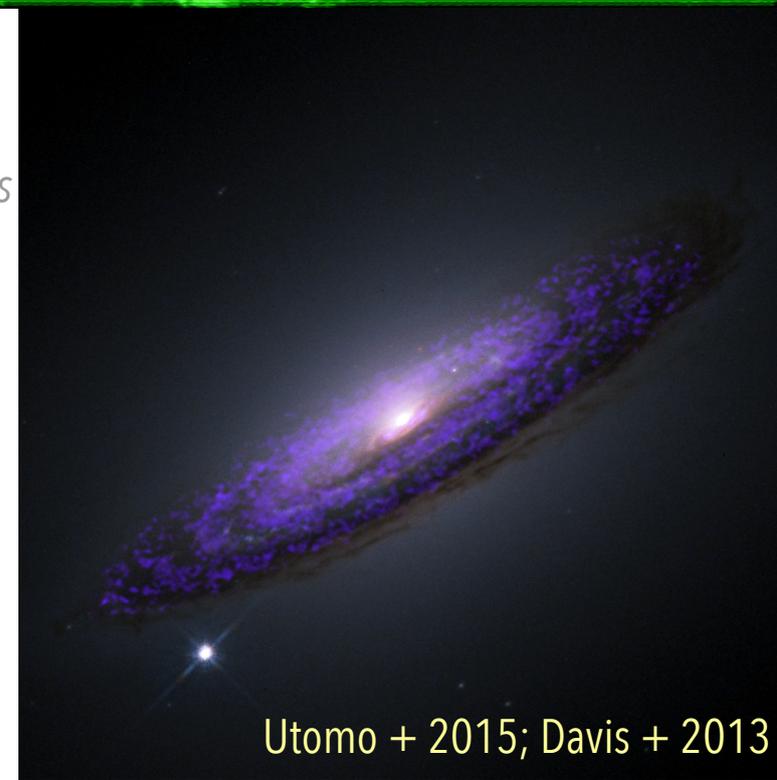
We recently published a paper in the journal "Nature" where we measured the mass of a super-massive black hole (in galaxy NGC4526) by tracing the motions of molecular gas clouds swirling around it (see Figure 1, next page). This technique is exciting, because it opens up the possibility of measuring black hole masses in more galaxies than ever before. The research paper describing this work has been published in Nature (February 15th 2013).

Super-Massive Black Holes

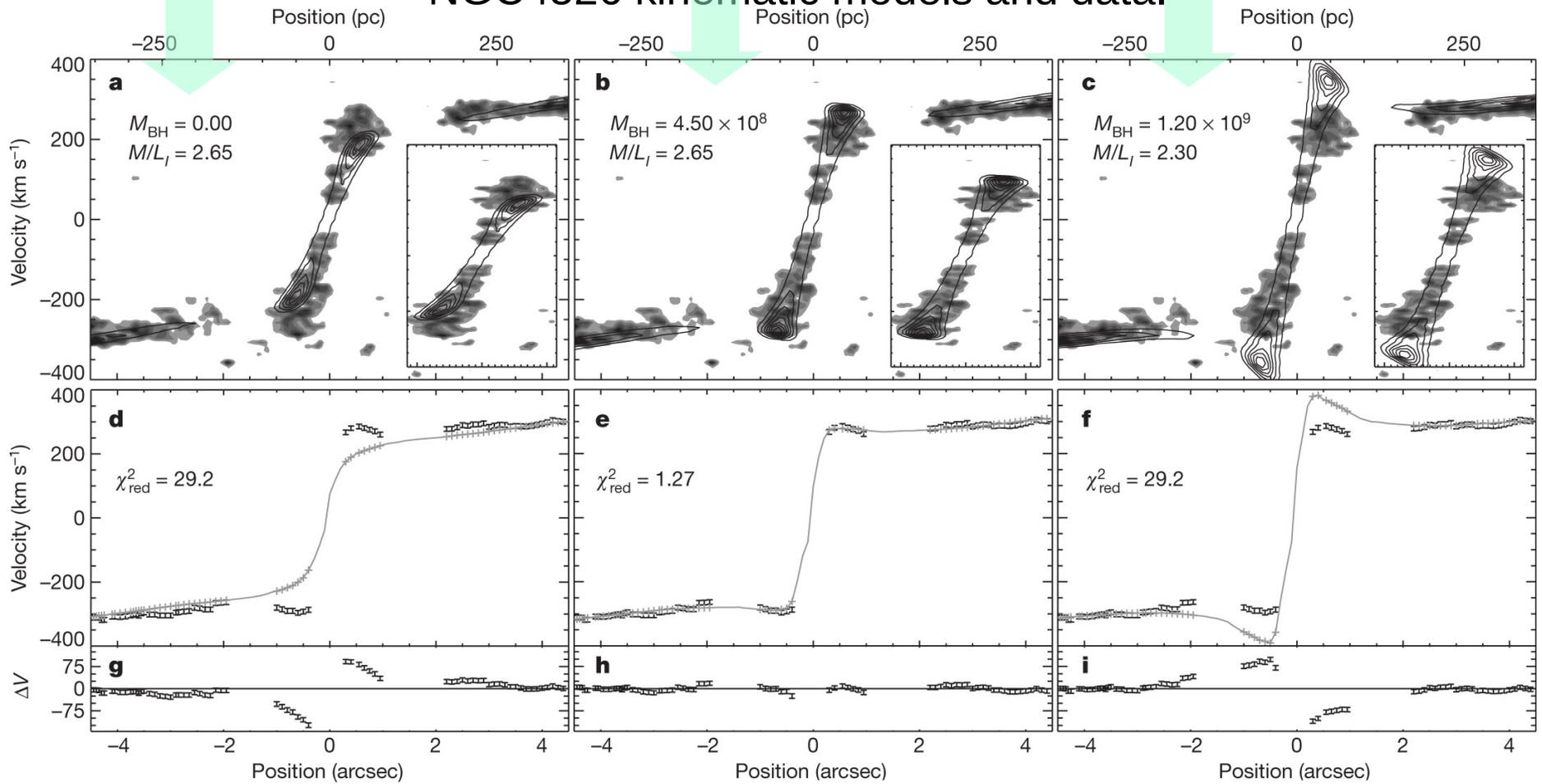
The masses of the super-massive black holes in the centres of galaxies appear to correlate with various properties of the parent galaxy (such as how bright the galaxy is, or the speed of random stellar motions). These relations extend from the biggest galaxies to small globular clusters, suggesting that there is a fundamental link between galaxy and black hole evolution. This is quite surprising, and not well understood, as these relations tie together quantities that probe very different length- and mass-scales.

These black hole correlations are based on a small number of black hole mass estimates, and the vast majority of the measurements have been made with just three methods. To understand the physical origin of the the black hole scaling relations we need more black hole mass measurements, and alternative techniques for measuring them.

The current methods for estimating black hole masses only work for relatively nearby galaxies, as you need to zoom in close to the black hole to measure its mass. Our paper demonstrates a new method for measuring black hole masses, with which we will be able to measure black hole masses much further out in the universe.



NGC4526 kinematic models and data.



TA Davis *et al.* *Nature* **000**, 1-3 (2013) doi:10.1038/nature11819

Molecular Gas Measurements

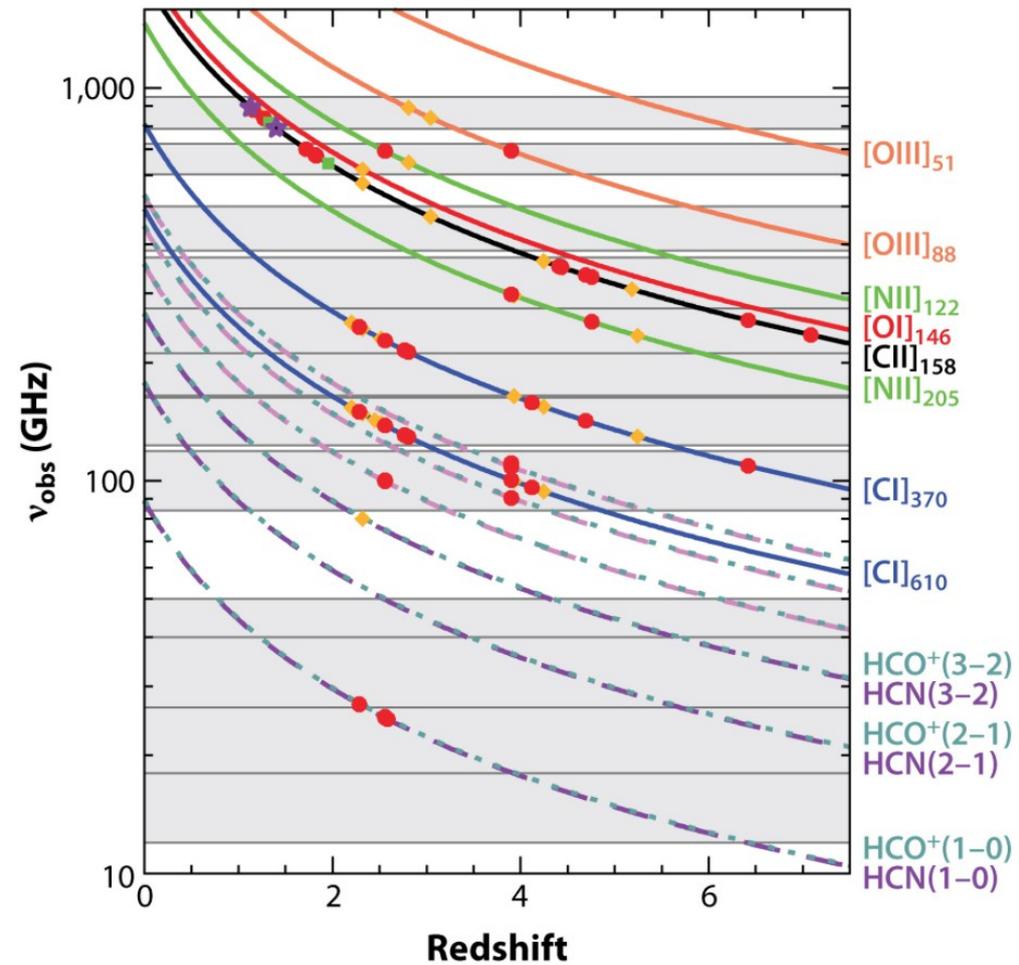
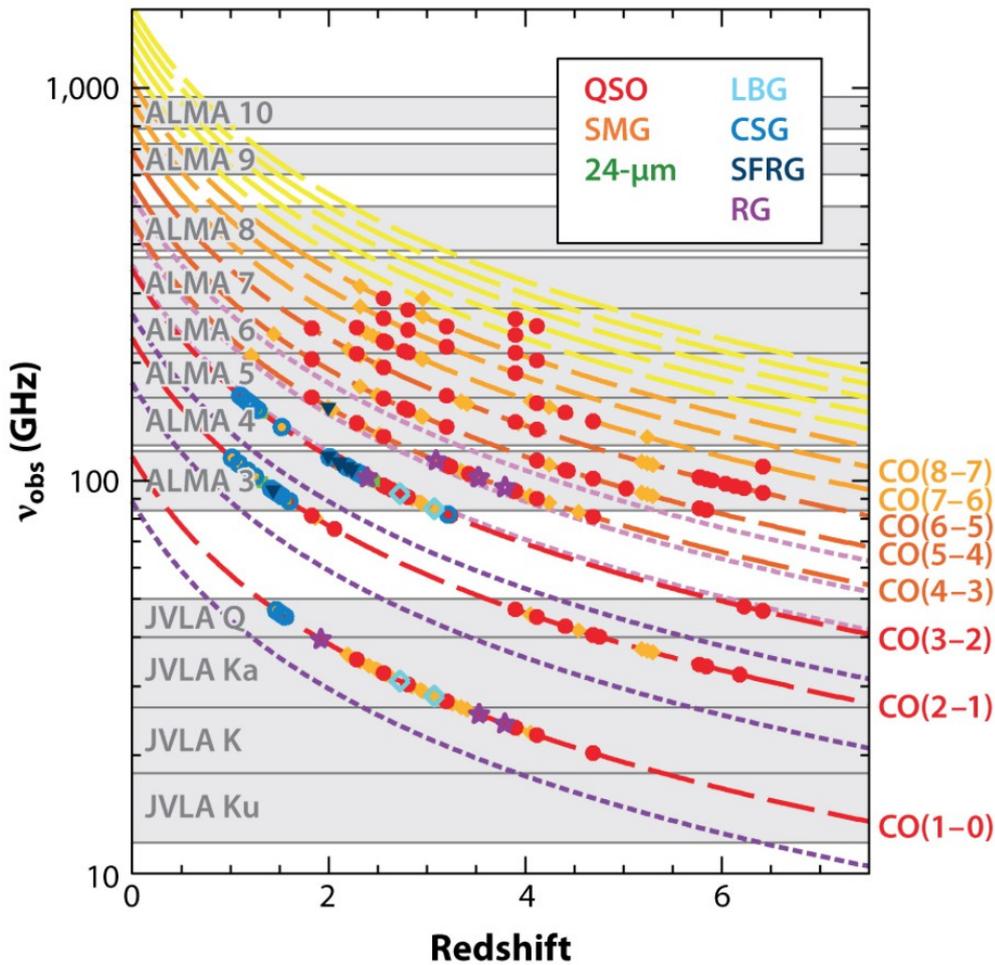
Molecules that we are familiar with in every day life also exist in space (however often in quite different proportions to those found on earth). The poisonous gas carbon monoxide is the second most abundant molecule in the universe. If we concentrated the gases in space to be as dense as our atmosphere, the result would be very toxic indeed! !

In this Nature paper, we observed carbon monoxide molecules in the galaxy NGC4526. We used the Combined Array for Research in Millimetre-wave Astronomy (CARMA) telescope (which you can see in Figure 3). CARMA uses an array of small dishes to obtain much sharper images than a single telescope could alone. This technique is called interferometry, and you can learn more about it here.

We observed NGC4526 with CARMA's sharpest array, achieving a resolution of 0.25 arcseconds. This is the equivalent of being able to spot a one euro coin (or US quarter) being held up 10 kilometres away! With these super sharp images we were able to zoom right into the centre of NGC4526, and observe the gas wizzing around the black hole. See the map of carbon monoxide in NGC4526 in Figure 1.

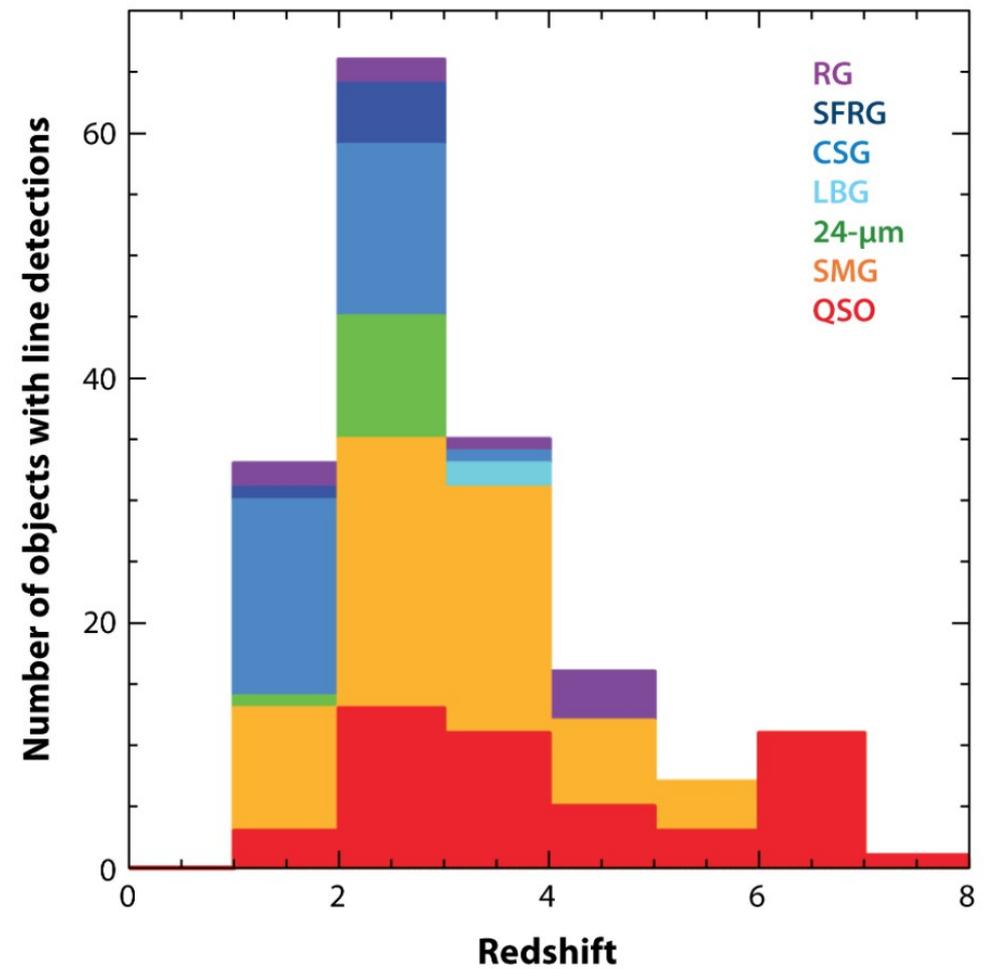
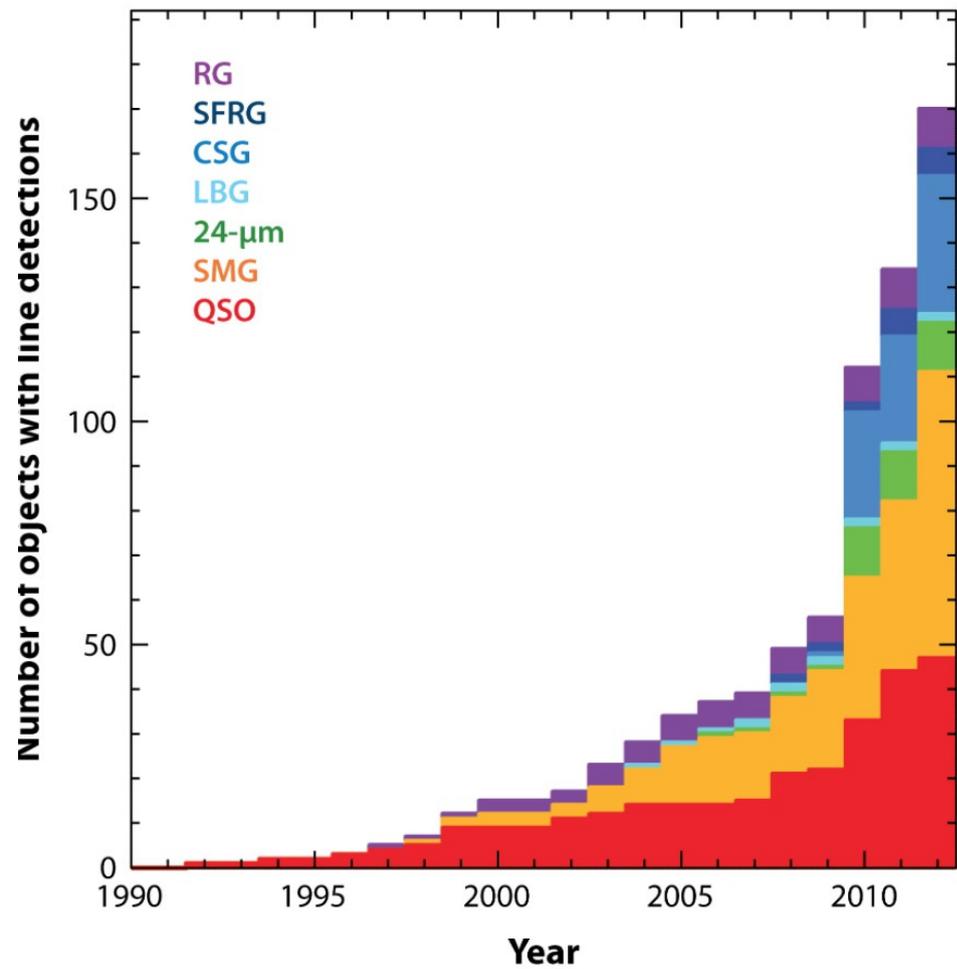
Gas (or any object) that orbits a black hole moves with a the speed that is determined by the mass of the black hole, and the distance from it. Our observations with CARMA give us the velocity of the gas at each position. Using this we were able to `weigh' the black hole in the centre of NGC4526, determining its mass.

Tracing reservoirs of cold gas in



AR Carilli CL, Walter F. 2013.
 Annu. Rev. Astron. Astrophys. 51:105–61

High redshift molecular gas



AR Carilli CL, Walter F. 2013.
Annu. Rev. Astron. Astrophys. 51:105–61

Tracing reservoirs of cold gas in (proto -) galaxies

Fuel for star formation and AGN activity (DIFFERENT SCALES!)

Star formation: --> infrared & UV emission, + radio, X-rays, etc

AGN: --> various phenomena: (optical) emission lines, UV & X-Rays, IR, radio emission, γ - rays

Observed in several hundreds Galaxies at $z > 1$ (out to $Z \sim 7$ in AGN)

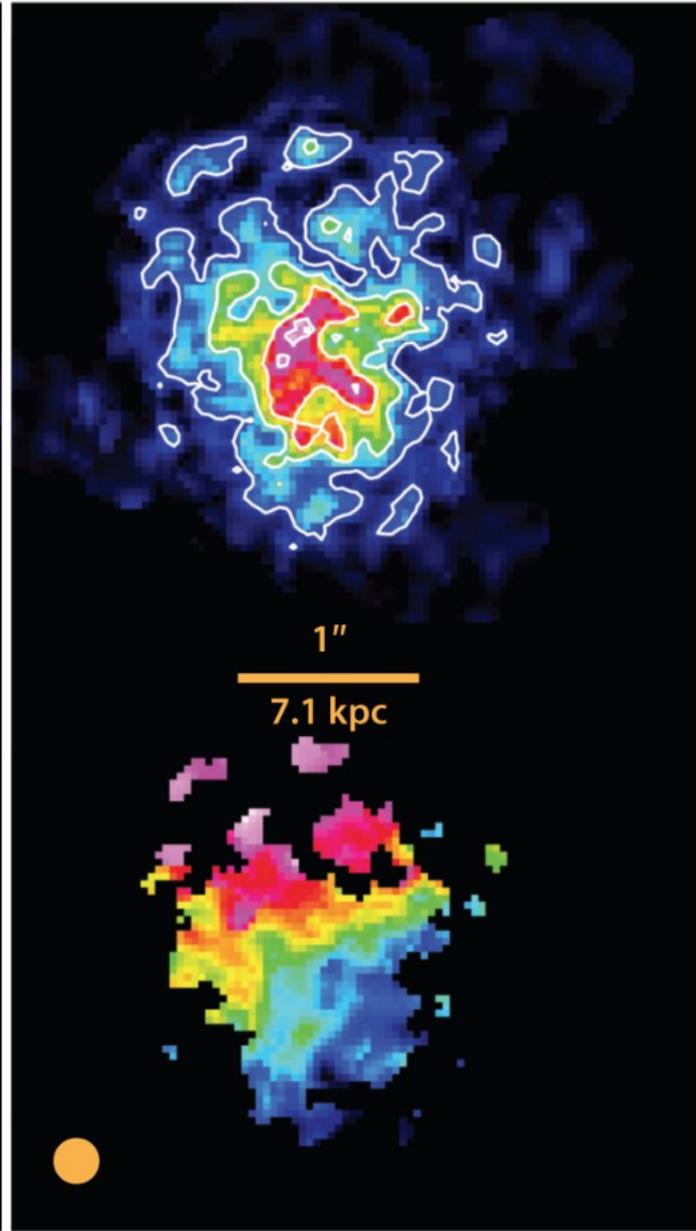
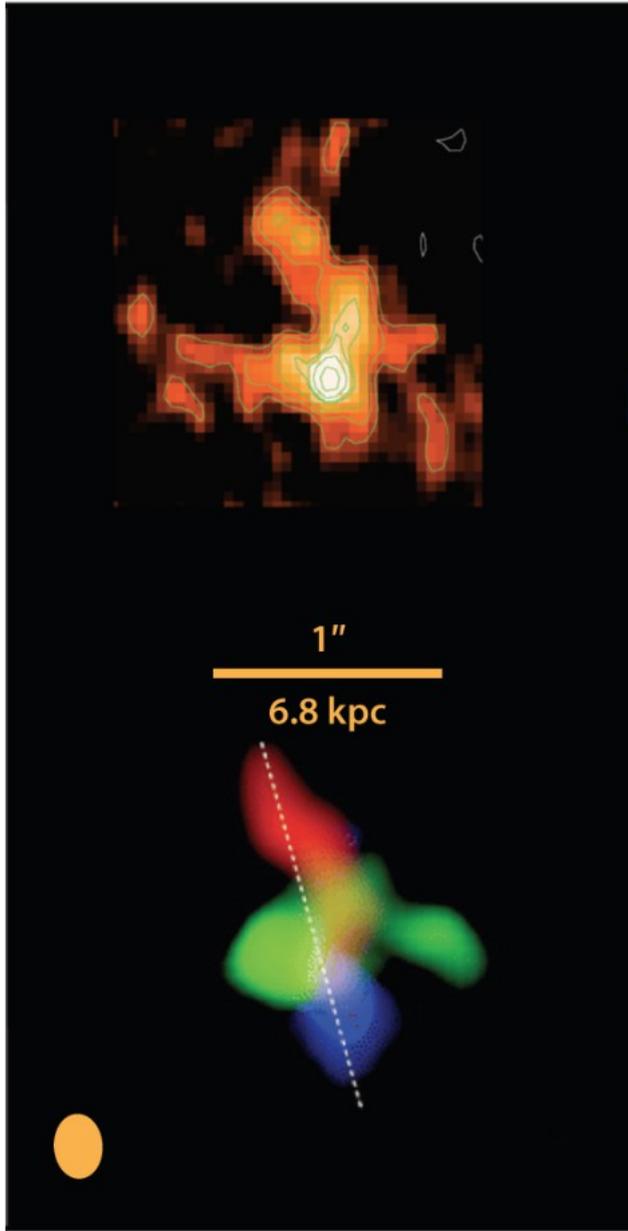
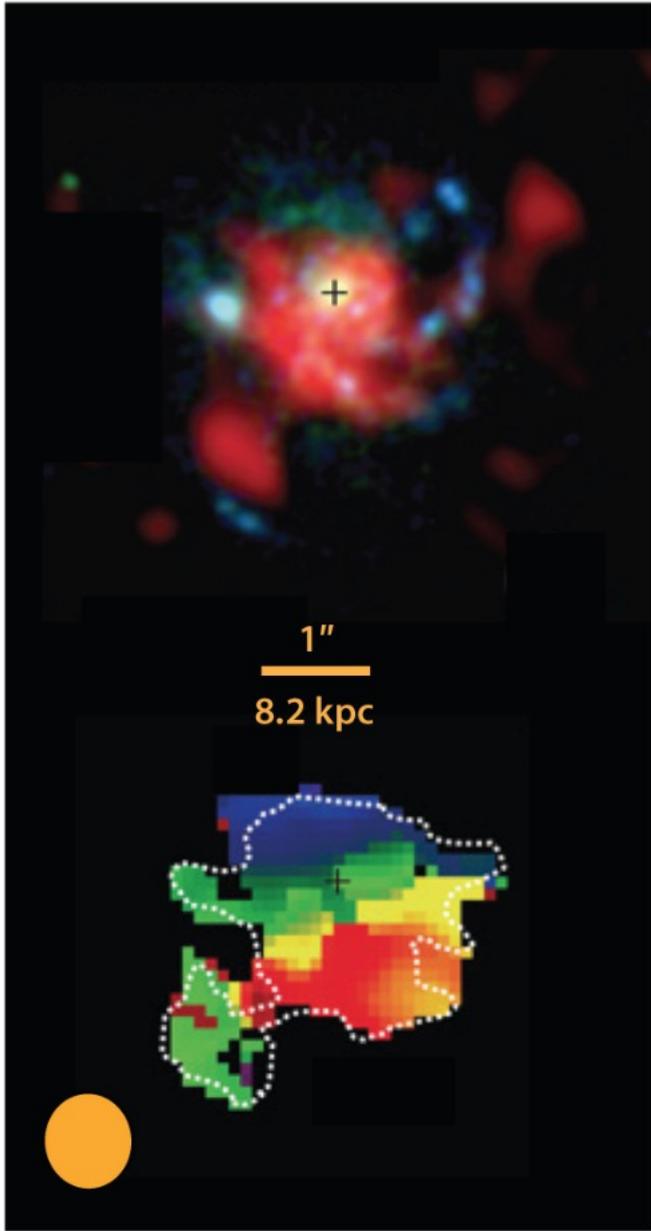
Gas is common in highly star-forming "sub-mm galaxies", particularly $1.5 < z < 2.5$

Is there a variation of X_{CO} .vs. z and .vs. galaxy type ?

Observational requirements:

Lines move in frequency (z dependent!), instruments become redshift windows

Integrated CO(2-1) map



Cold (molecular) gas is found in form of molecules associated with DUST (helps formation, shields from high energy radiation)

- *Homologous molecules do not have electric dipole, high energy transitions in very particular physical conditions (high T, high P), i.e. rare!*
- *CO, despite its low electric dipole is commonly seen, being the second to H₂ in abundance
At typical ISM conditions J1 → 0 is weaker than higher (J → J-1) transitions, and it is optically thick when $n > 2000 \text{ cm}^{-3}$*
- *Gas in all phases is found in Spiral & Irregular galaxies, most evident in interacting objects
Thin disk distribution, avoids the bulge, and the outer parts (density is too low!)*
- *Little or no cold gas is found in elliptical and S0 galaxies, with a few exceptions*
- *Gas condensations create conditions for (intense) star formation*

Observability of H₂ emission

- Molecular hydrogen is a symmetric molecule
 - The electric dipole moment is zero
 - Rotational transitions are forbidden, even though electronic transitions are allowed
- Quadrupole transitions are possible
 - They are very weak and characterized by energies much higher than the typical rotational energies
 - Can only be observed in relatively warm regions

Thanks to the abundance of H₂ some of these transitions have been observed in the mid IR

- Lack of H₂ emissions \Rightarrow hard to make maps of the distribution of molecular hydrogen
 - UV absorptions require (rare) bright background sources and are not suited to make maps, especially in regions rich of dust and molecules, where the background sources are obscured

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Species	Transition	Lambda (mu)	E_l (cm-1)	Reference
H2	(1,0) Q(1)	2.4065914	118.49	Bragg et al. 1982
H2	(2,1) Q(1)	2.5510	118.49	Black & van Dishoeck 1987
H2	(2,1) Q(3)	2.5698	705.52	Black & van Dishoeck 1987
H2	(2,1) Q(5)	2.6040	1740.24	Black & van Dishoeck 1987
H2	(1,0) O(2)	2.6269	354.37	Black & van Dishoeck 1987
H2	(1,0) O(3)	2.8025	705.52	Black & van Dishoeck 1987
H2	(1,0) O(5)	3.2350	1740.24	Black & van Dishoeck 1987
H2	(0,0) S(13)	3.8468	9580.75	Jennings et al. 1985 constants
H2	(0,0) S(11)	4.1813	7148.71	Jennings et al. 1985 constants
H2	(0,0) S(10)	4.4099	6039.15	Jennings et al. 1985 constants
H2	(0,0) S(9)	4.69461	5005.73	Jennings et al. 1987
H2	(0,0) S(8)	5.05303	4053.51	Jennings et al. 1987
H2	(0,0) S(7)	5.51116	3188.05	Jennings et al. 1987
H2	(0,0) S(6)	6.10856	2415.08	Jennings et al. 1987
H2	(0,0) S(5)	6.90952	1740.24	Jennings et al. 1987
H2	(0,0) S(4)	8.02505	1168.81	Jennings et al. 1987
H2	(0,0) S(3)	9.66491	705.52	Jennings et al. 1987
HD	(0,0) R(10)	11.57346	4627.07	Ulivi et al. 1991
H2	(0,0) S(2)	12.27861	354.37	Jennings et al. 1987
HD	(0,0) R(9)	12.47181	3825.27	Ulivi et al. 1991
HD	(0,0) R(8)	13.59265	3089.58	Ulivi et al. 1991
HD	(0,0) R(7)	15.25104	2423.88	Ulivi et al. 1991
HD	(0,0) R(6)	16.89381	1831.95	Ulivi et al. 1991
H2	(0,0) S(1)	17.03483	118.49	Jennings et al. 1987 <- lowest energy, corresponding to T_excitation ~ 850 K
p-H2O	5_51-4_04	19.2300	222.05	HITRAN
HD	(0,0) R(5)	19.43100	1317.31	Ulivi et al. 1991
o-H2O	5_50-4_23	22.6391	300.36	HITRAN
HD	(0,0) R(4)	23.03376	883.16	Ulivi et al. 1991
OH 1/2-3/2	9/2-7/2	24.614	201.93	Offer & van Dishoeck 1992
OH 1/2-3/2	9/2-7/2	24.642	202.38	Offer & van Dishoeck 1992
o-H2O	5_41-4_14	25.9402	224.84	HITRAN

Estimating the excitation temperature,
in K, of a given transition (using MKs units)

$$T = \frac{h\nu}{k} = \frac{hc}{\lambda k} = \frac{6.626 \cdot 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{1.38 \cdot 10^{-23} \text{ kg m}^2 \text{ s}^{-2} \text{ K}^{-1}} \nu = 4.80 \cdot 10^{-11} \nu = 4.80 \cdot 10^{-11} \frac{c}{\lambda} \quad [\text{K}]$$