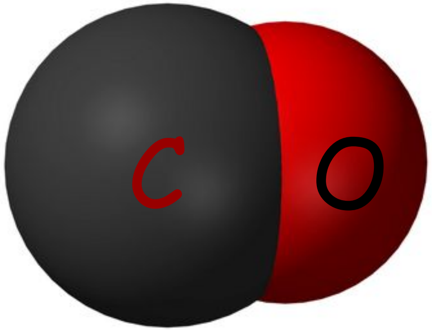
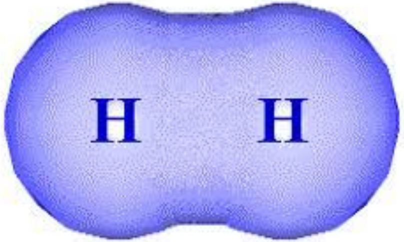
# Different Mechanisms for Molecular Spectral Line Emission

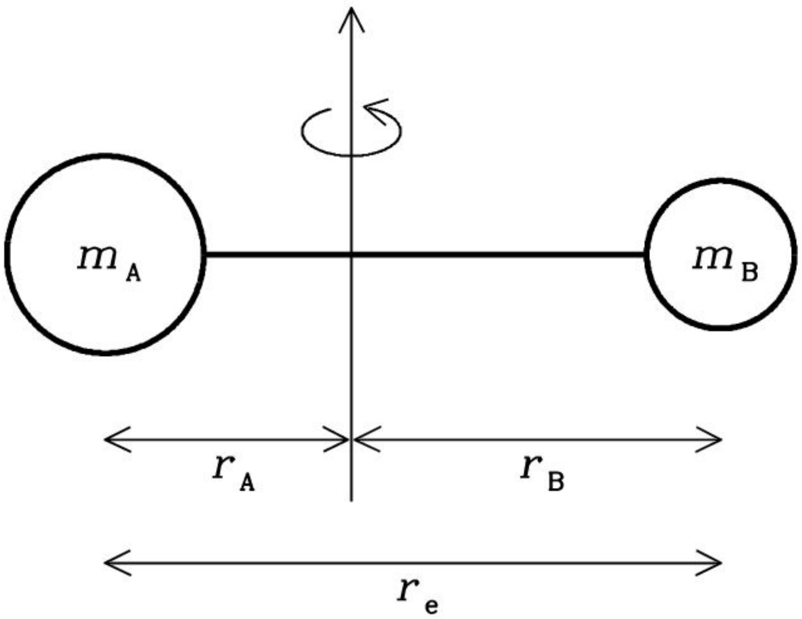



1. Rotational Lines
   a. I.E. Radio CO Lines
2. Vibrational Lines
   a. I.E. Radio $NH_3$
3. Roto-vibrational Lines
   a. UV emission of $H_2$


**Their strength is intrinsically tied to molecular structure, and the kinetics of molecules.**

# Simplest Example: Rotational Lines of the CO Molecule




A simple dumbbell like model for the derivation of the rotational frequencies.

# Quantized orbital momentum in a Bohr-like atom:

$$L = m_e v r$$

r is the allowed orbital radius for the Bohr atom.

$$= m_e v a_n$$

$a_n = (n\hbar) \times (m_e v)^{-1}$

$$= (m_e v) \times (n\hbar) \times (m_e v)^{-1}$$

$$= \boxed{n\hbar}$$

# Quantized Energy from Quantized Momentum:

$E_{rot} = (I\omega^2) \times (2)^{-1}$

$L = I\omega$

$= (L^2) \times (2I)^{-1}$

Energy eigenvalues for $L^2$ are $\hbar^2 J(J+1)$

$= (\hbar^2 J(J+1)) \times (2I)^{-1}$

$I = \mu r_e^2$ , $\mu$ is the usual reduced mass.

$$= (\hbar^2 J(J+1)) \times (2\mu r_e^2)^{-1}$$

# Transitions between two levels:

$$\Delta E = ([(J+1)J - J(J-1)]\hbar^2) x (2\mu r_e^2)^{-1}$$

$$= (2J\hbar^2) x (2\mu r_e^2)^{-1}$$

$$= (Jh^2) x (4\pi^2\mu r_e^2)^{-1}$$

ΔJ must be equal to ±1 due to quantum mechanical selection rules for allowed transitions.

$\hbar = h/(2\pi)$

# Simplest Example: Rotational Lines of the CO Molecule

$$\nu_{obs} = \Delta E/h$$

$$\nu_{obs} = (hJ)x\,(4\pi^2\mu r_e^{2})^{-1} \text{ for } J = 1,2,3,..$$

For $^{12}C^{16}O$ "normal CO"

:

$\mu \cong 1.15e\text{-}23g$

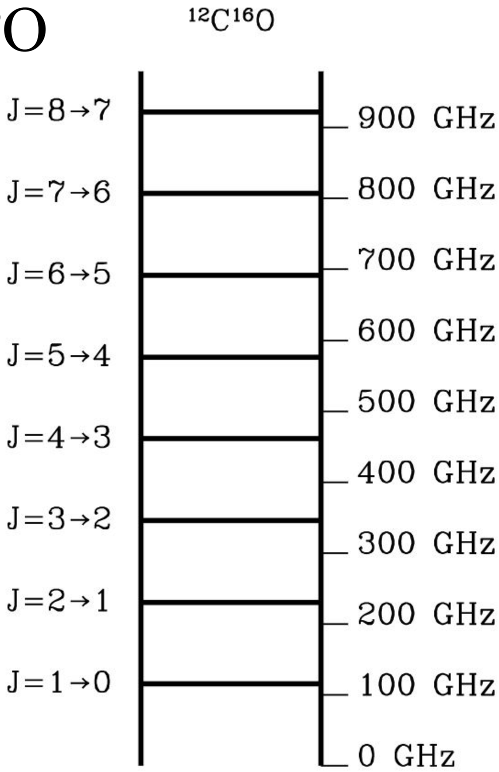
$r_e \cong 1.13e\text{-}8cm$

→

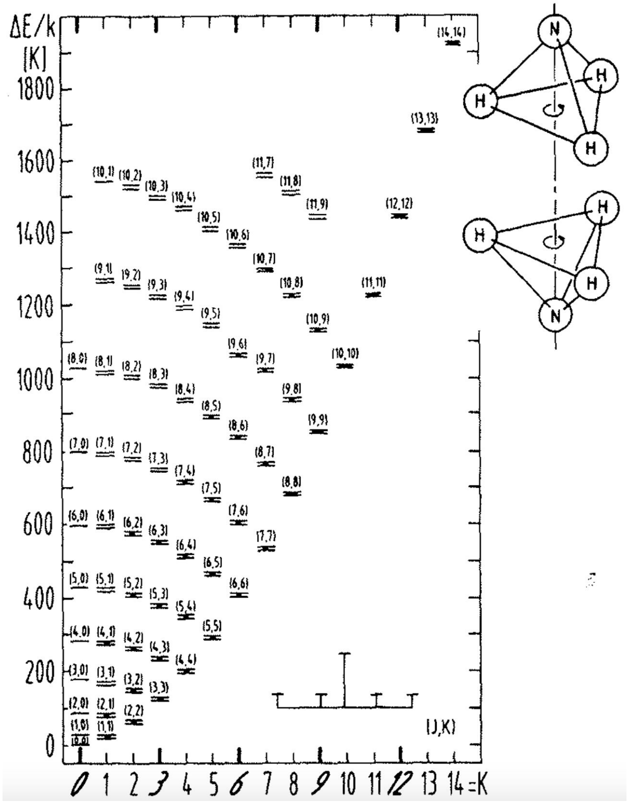
$$\nu_{obs} = 115.271 \text{ GHz}$$

# Simple vs. Complex Vibrational line spectra

$^{12}C^{16}O$




$NH_3$



# Isotopologues*

**Definition:** Molecules that have identical structure and atomic composition but contain different isotopes, effectively meaning there are different numbers of neutrons.

**Example:** $^{12}C^{16}O$, $^{13}C^{16}O$, $^{13}C^{18}O$

*My favorite chemistry word.

# Isotopologues Emission:

$$[\nu_{1\text{-}0}(^{13}C^{16}O)]x[m(^{13}C^{16}O)] = [\nu_{1\text{-}0}(^{12}C^{16}O)]x[m(^{12}C^{16}O)]$$

This allows for an easy calculation of the emitting frequency for different isotopologues.

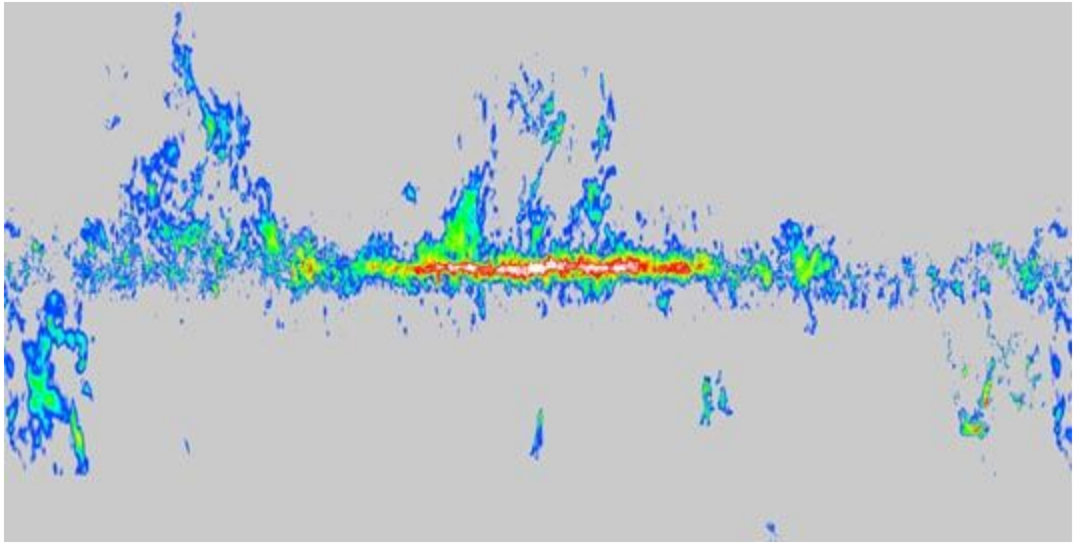
# Practice Problem:

The lowest observable frequency with ALMA is 84 GHz. What is the lowest $^{12}C^{16}O$ transition ALMA can detect for a galaxy at redshift 2?

Pertinent Information:

1. Assume $^{12}C^{16}O$ J = 1-0 transition is at 115 GHz.
2. Recall that $z = (\nu_{em}/\nu_{obs}) - 1$

# Molecular Lines in Galaxies



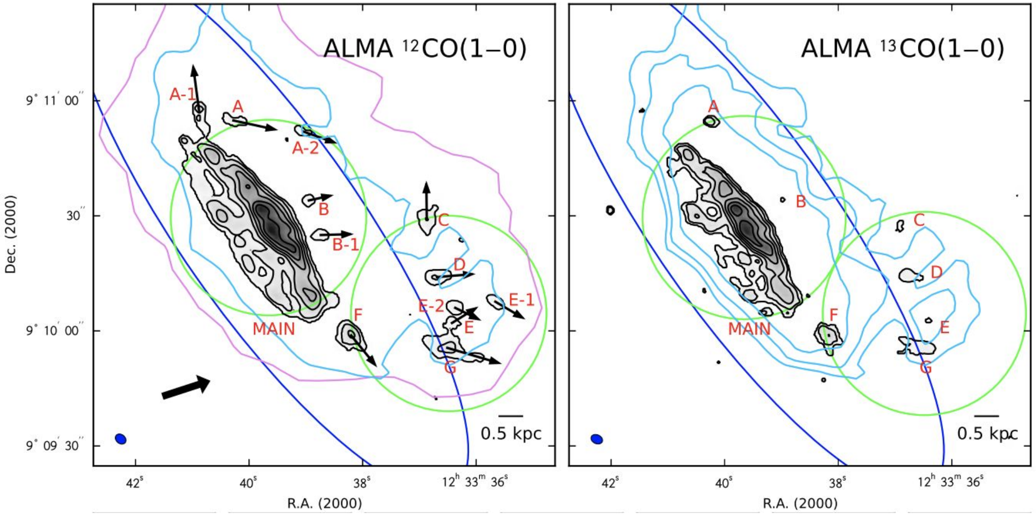
**Milky Way Molecule Map: Credit:** T. Dame (CfA, Harvard) et al., Columbia 1.2-m Radio Telescopes

CO is an important tracer of star formation, and is often assumed to be correlated with the amount of the unobservable $H_2$.

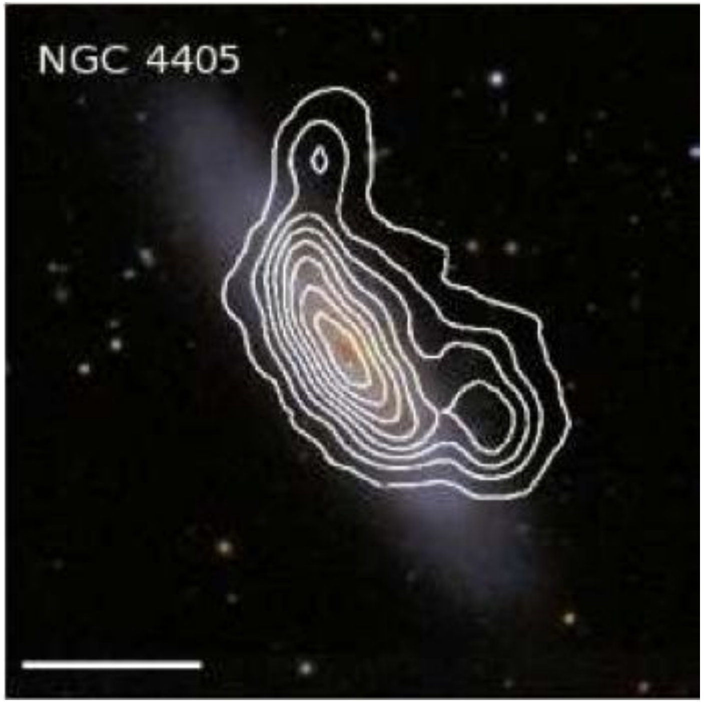
The conversion between CO column density and $H_2$ mass.

$X_{CO} \cong 2e20\ cm^{-2}\ (K\ km/s)^{-1}$

# CO in NGC 4522

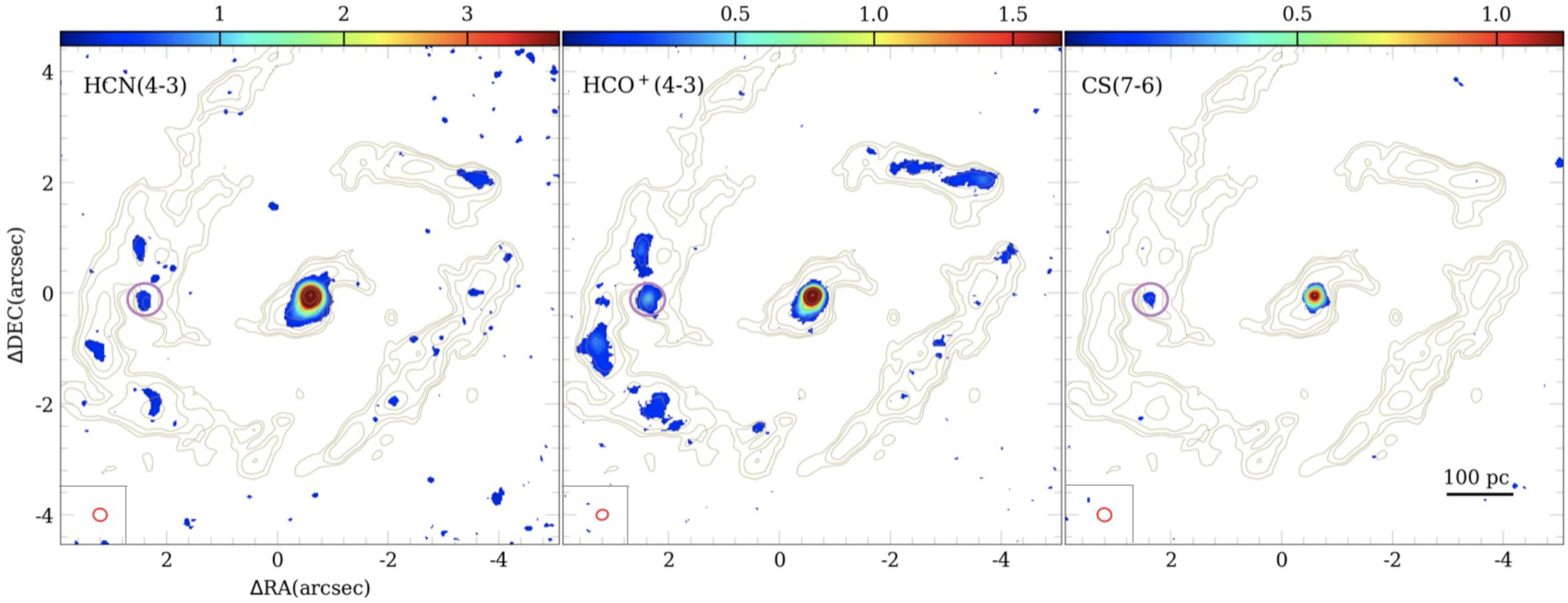



Blue and pink contours are HI and greyscale and contours are CO. **Credit:** *Lee, Bumhyun, Chung, Aeree, 2018, ApJ, The ALMA Detection of Extraplanar 13CO in a Ram-pressure-stripped Galaxy and Its Implication*




HI over optical galaxy. Credit: VIVA HI Imaging Survey 2009.

# Molecular Lines and Supermassive Black Holes




Different molecules overlaid on CO contours around a supermassive black hole. **Credit** *A. Audibert et al.: ALMA captures feeding and feedback from the active galactic nucleus in NGC 613*