



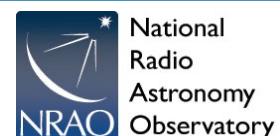
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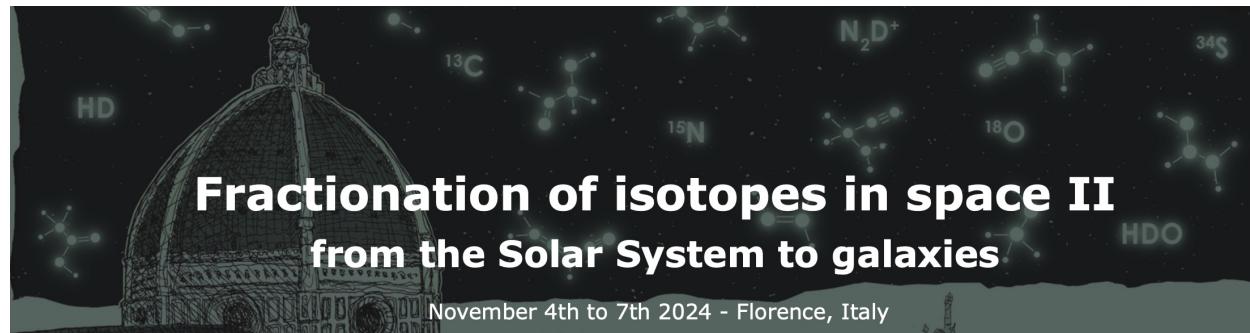
**Department of  
Physics and  
Astronomy**

Galileo Galilei  
Institute for  
Theoretical Physics



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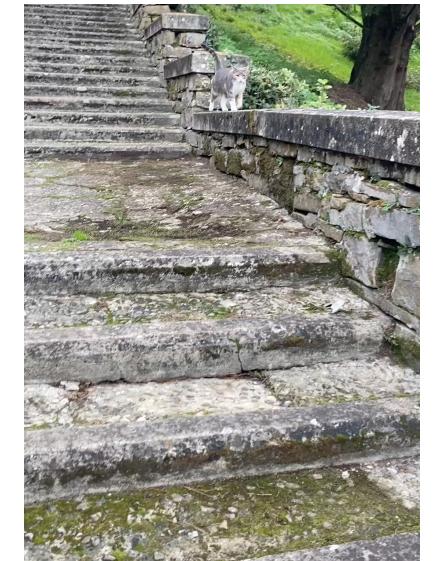




Views!

Foods!

Cats!



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# Emission Mechanisms

Spectral Lines (ERA Chap. 7)



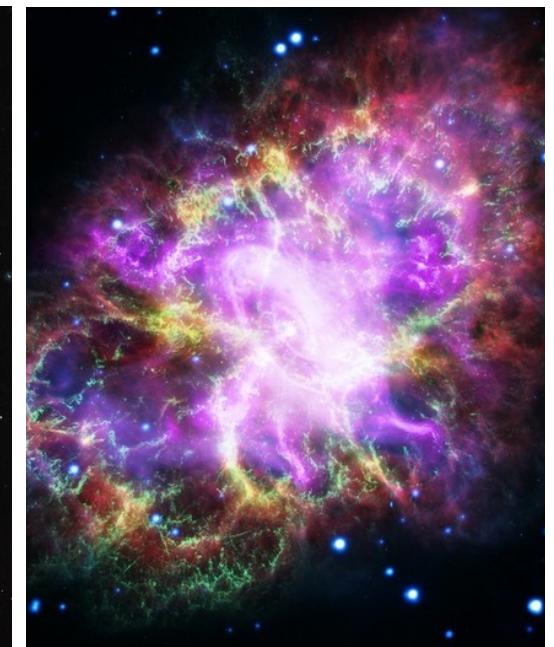
Free-Free (ERA Chap. 4)



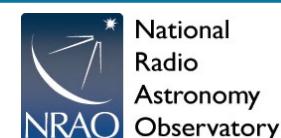
Synchrotron (ERA Chap. 5)



Pulsars (ERA Chap. 6)



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# Emission Mechanisms

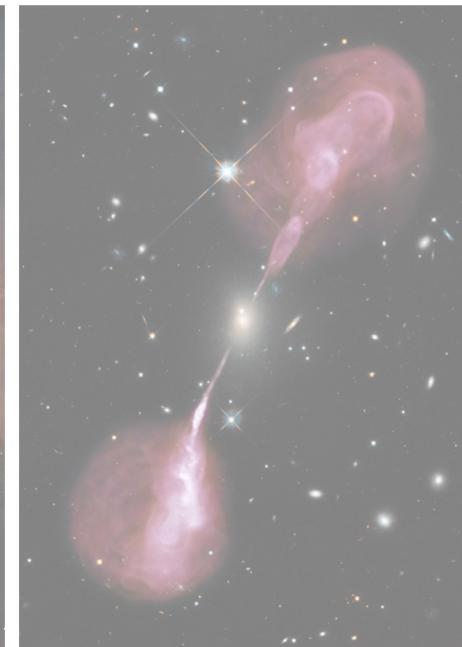
Spectral Lines (ERA Chap. 7)



Free-Free (ERA Chap. 4)



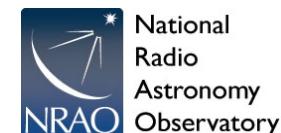
Synchrotron (ERA Chap. 5)



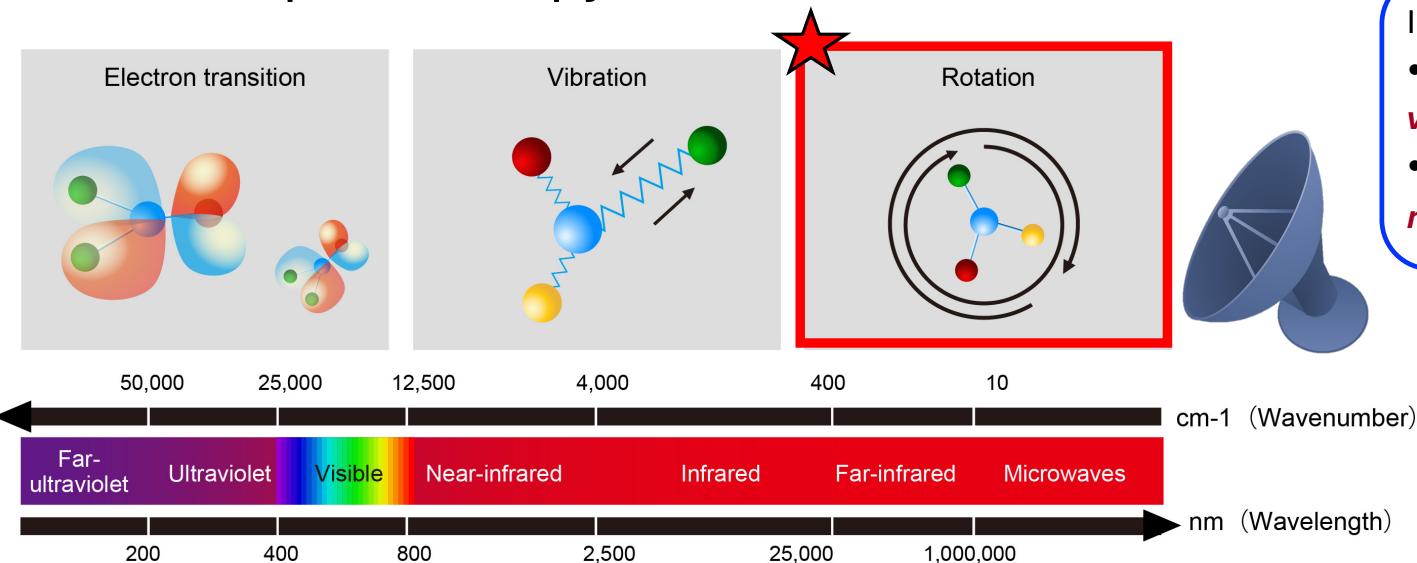
Pulsars (ERA Chap. 6)



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# Submillimeter and Millimeter Radio Telescopes Identify Molecules via Rotational Spectroscopy!



## 1) ELECTRONIC STATES

- electrons change levels
- energies in visible, UV

## 2) VIBRATIONAL STATES

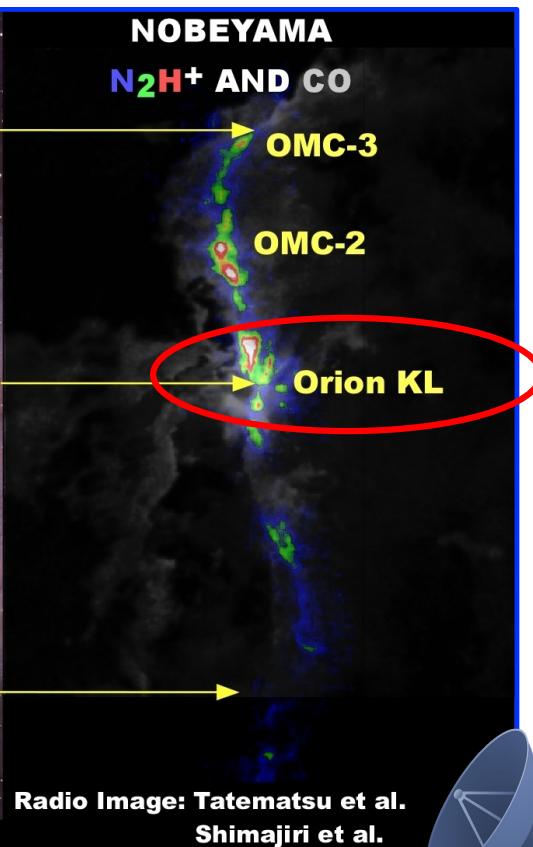
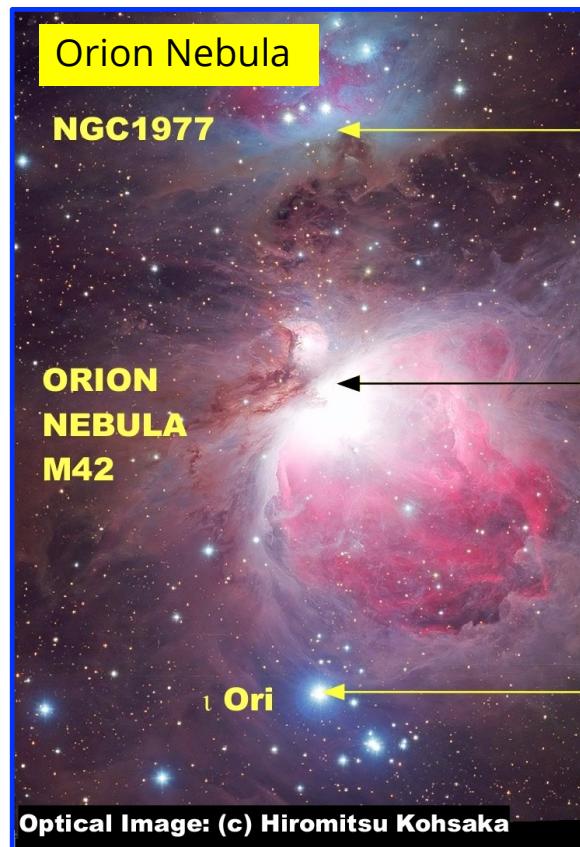
- normal modes of nuclear motions
- occur in infrared region

## 3) ROTATIONAL STATES

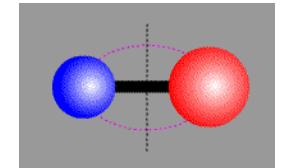
- end-on-end motion of nuclei
- energies in microwave/millimeter-wave regions

Important to know all because...

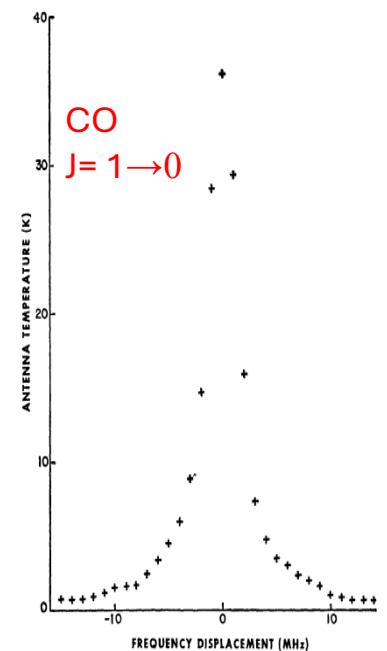
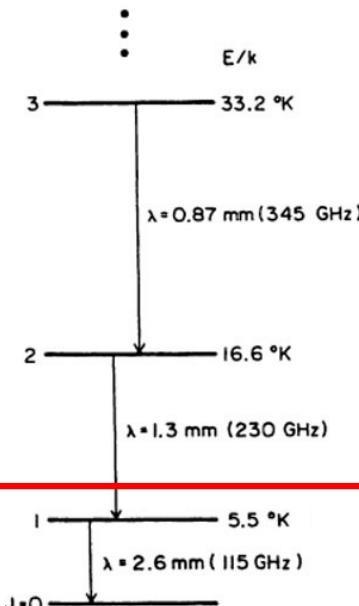
- Electronic states have **vibrational/rotational structure**
- Vibrational states have **rotational structure**



**Discovery of CO**  
in the Star Forming Region,  
Orion KL at 115 GHz  
( $J = 1 \rightarrow 0$  transition)  
in 1970 at Kitt Peak, Arizona!



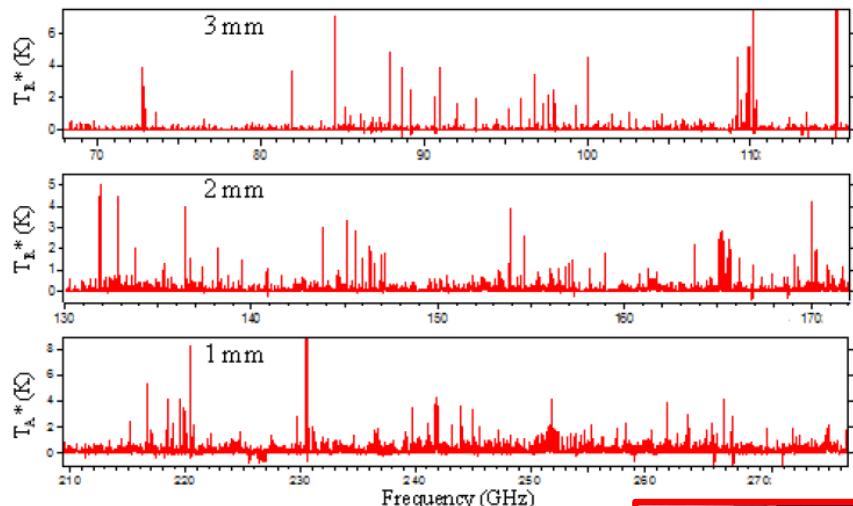
#### CO Rotational Levels



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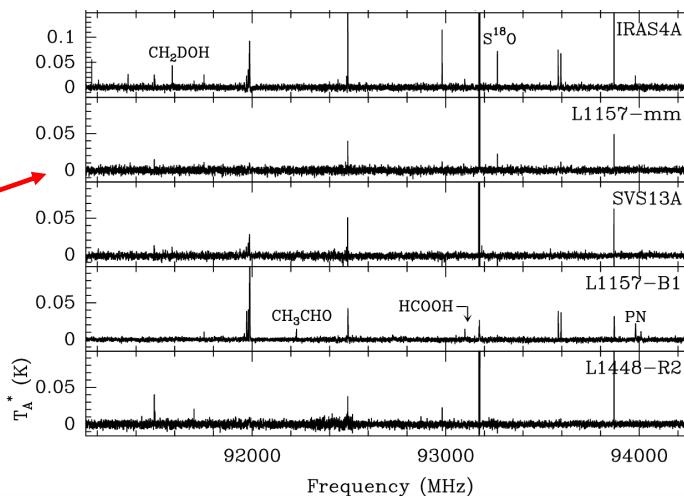


# Rotational Lines of Molecules at Radio Wavelengths



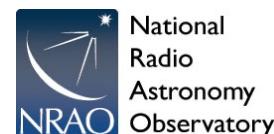
Credit: L. Ziurys

- We look at the **excitation conditions** of a molecule to know what to look for
- We use **radiative transfer** to calculate physical parameters, such as column densities and masses



Lefloch 2018

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## Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

### \*Key Things to Remember!

**Excitation Temperature** is defined by the **Boltzmann equation** and gives the ratio of the populations in each level ( $T_{ex}$  or  $T_x$ ):

$$T_{ex} = \frac{h\nu/k}{\ln \frac{n_l g_u}{n_u g_l}},$$

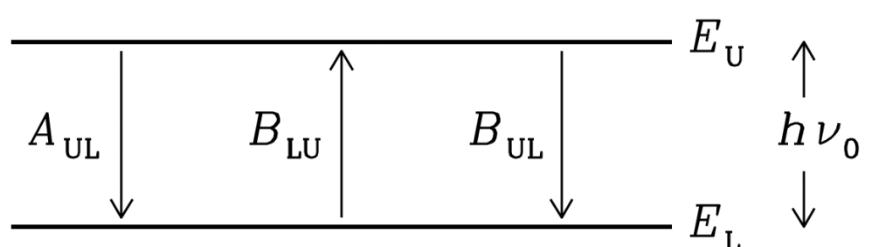
\* When  $T_{ex} \sim T_k$  then LTE a good approximation!

Optically thick lines (e.g.,  $^{12}\text{CO}$ ) or dust emission can be used to determine the **temperature** of a cloud!

Optically thin lines (e.g.,  $^{13}\text{CO}$  or  $\text{C}^{18}\text{O}$ ) or dust emission is directly proportional to the **cloud's optical depth** (and thus column density and cloud mass)!

To get column density,  $N_L$ , you need to know the physical states of your molecule and calculate the spontaneous emission coefficient

Fig. 7.5 (ERA)



In practice... we look up these terms in Splatatalogue!

<https://splatalogue.online>

## Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

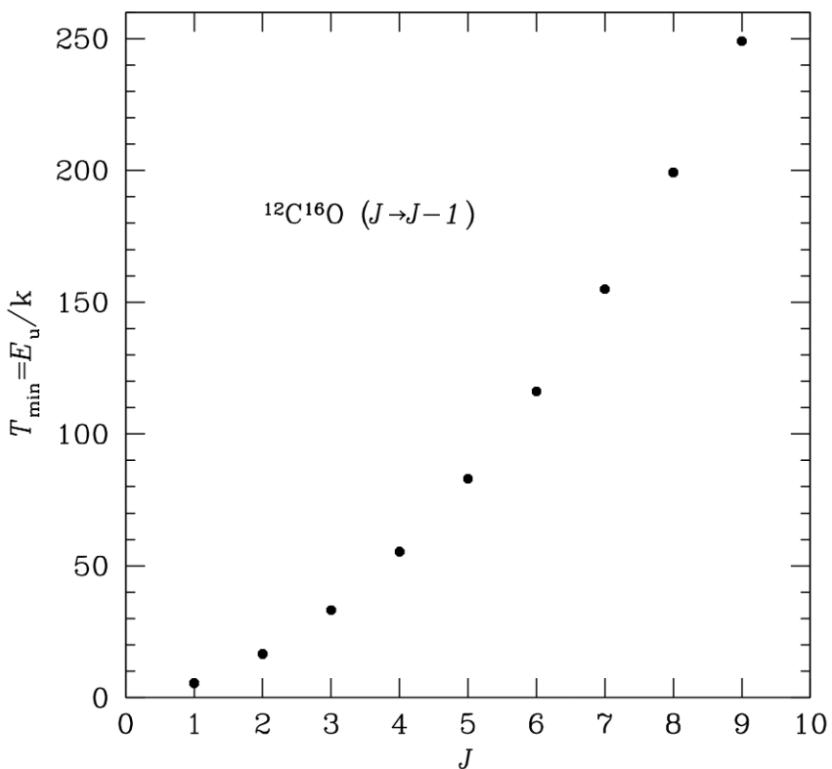
### \*Key Things to Remember!

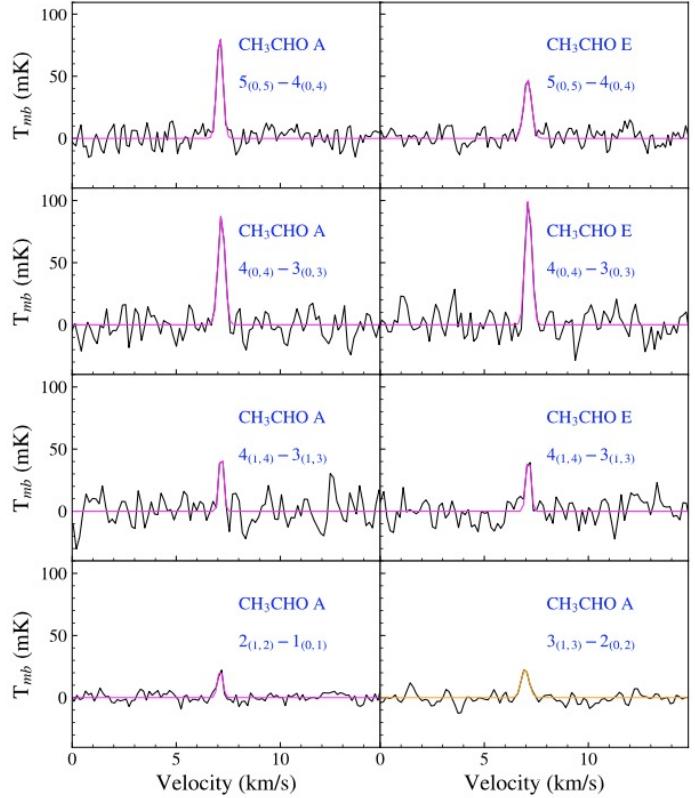
Related to  $A_{UL}$ , the **upper energies** give clues into what type of environments are molecular lines are likely to emit at and are directly connected to the minimum gas temperature needed for significant collisional excitation,

$$T_{\min} \sim \frac{E_{\text{rot}}}{k}$$

$$\sim \frac{J(J+1)h^2}{2 \cdot 4\pi^2Ik} = \frac{hJ}{4\pi^2I} \frac{h(J+1)}{2k} = \frac{E_U}{k}$$

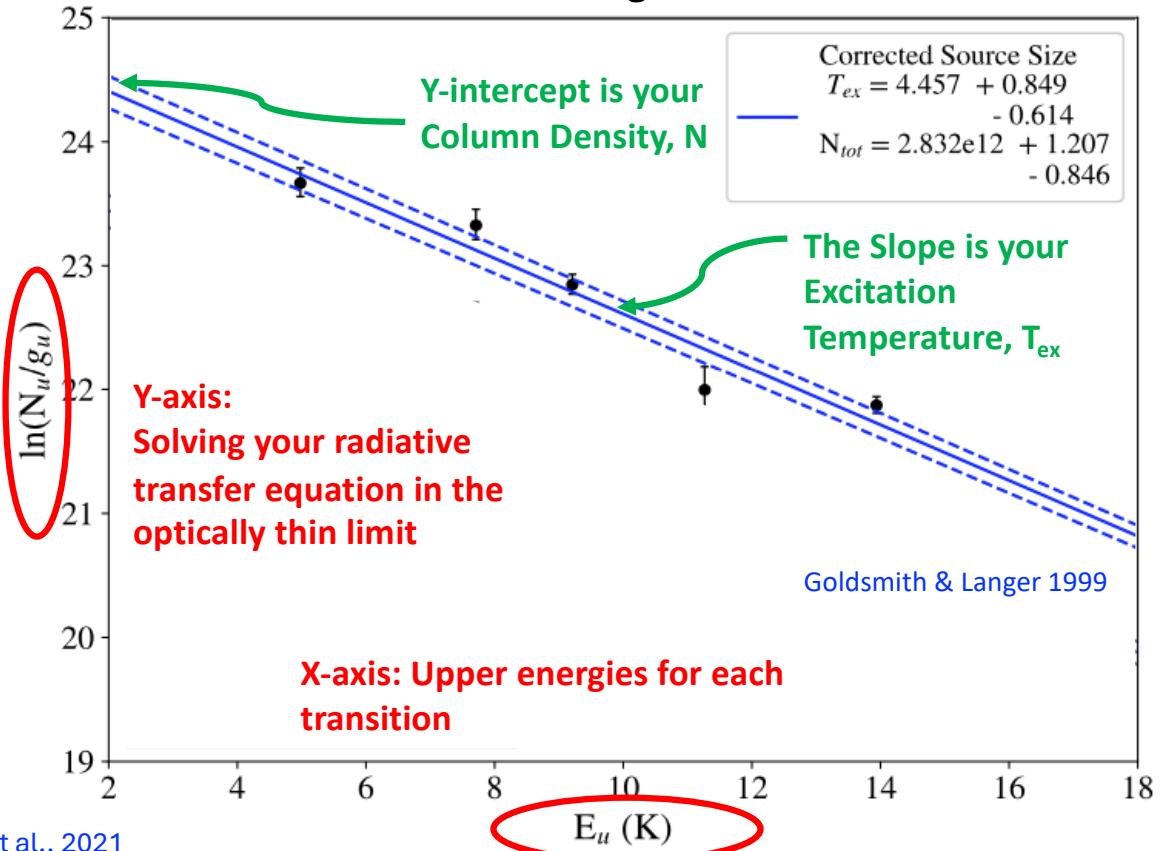
(7.116 & 7.118)





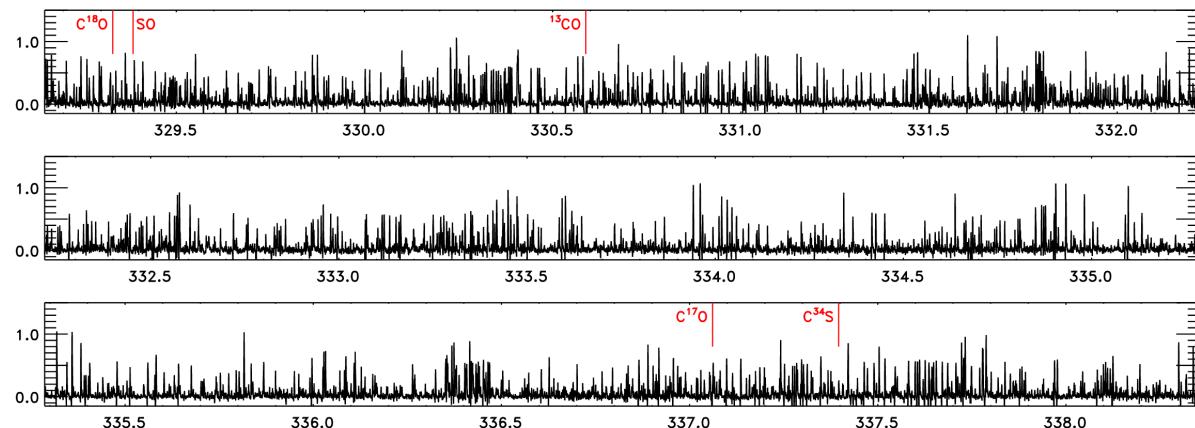
Scibelli et al., 2021

### Practical use → Rotation Diagrams



## Isotopologues (ERA 7.7)

**"Molecules that differ only in isotopic composition; that is, only in the numbers of neutrons in their component atoms"**



Jørgensen et al. 2016

**"The process called isotopic fractionation comes into play when it becomes energetically favorable to substitute an abundant isotope with a less abundant one"**

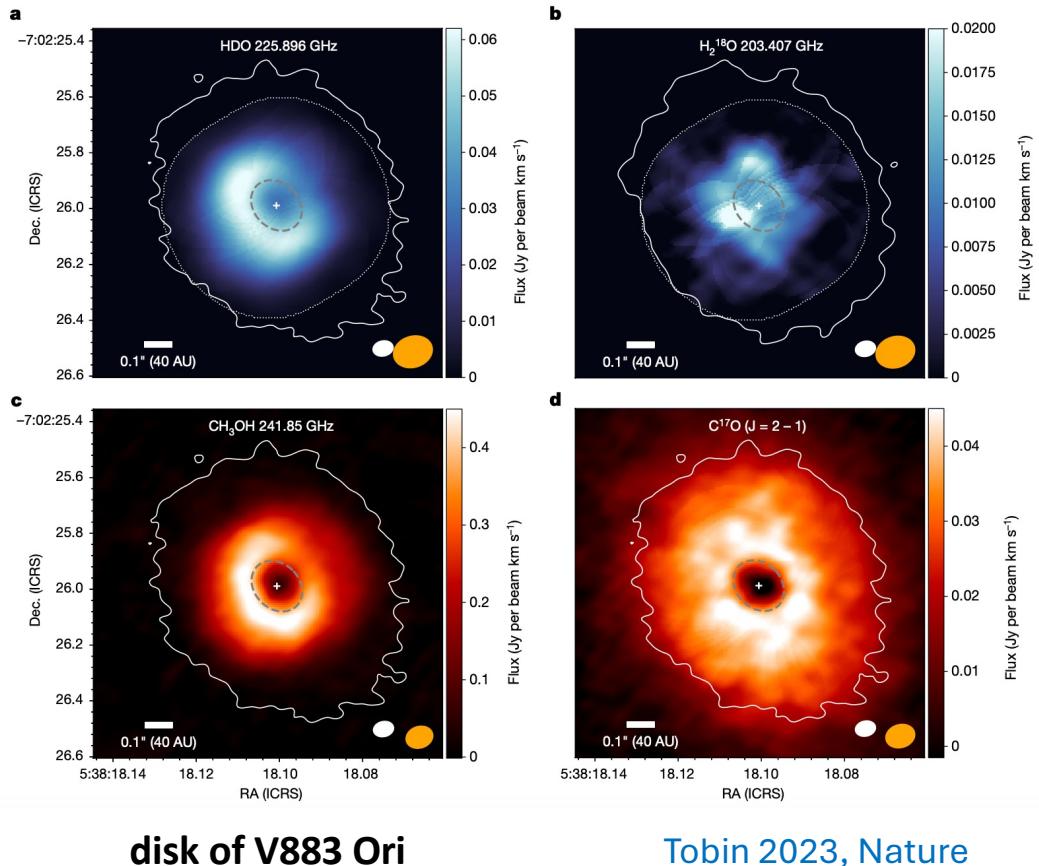
E.g.,

$\text{C}^{18}\text{O}$ ,  $\text{C}^{13}\text{CO}$ ,  $\text{C}^{17}\text{O}$ ,  $\text{C}^{34}\text{S}$ ,  $\text{H}^{13}\text{CO}^+$ ,  $\text{HC}^{18}\text{O}^+$ ,  $\text{H}^{13}\text{CN}$ ,  $\text{H}^{15}\text{CN}$ ,  $\text{Si}^{29}\text{O}$ ,  $\text{CH}_3\text{OH}^{13}$ , DCN, DCO $^+$

## Isotopologues (ERA 7.7)

Benefits of observing Isotopes:

- **Usually optically thin lines**
  - Therefore can be used to measure the column densities needed to estimate the total mass of molecular gas in a source
  - Intensity ratios of optically thin lines from different J levels can be used to measure excitation temperature, which is close to the kinetic temperature in LTE
- **\*Chemical ‘clocks’ that can age molecular clouds and trace the chemical evolution\***



## Isotopologues (ERA 7.7)

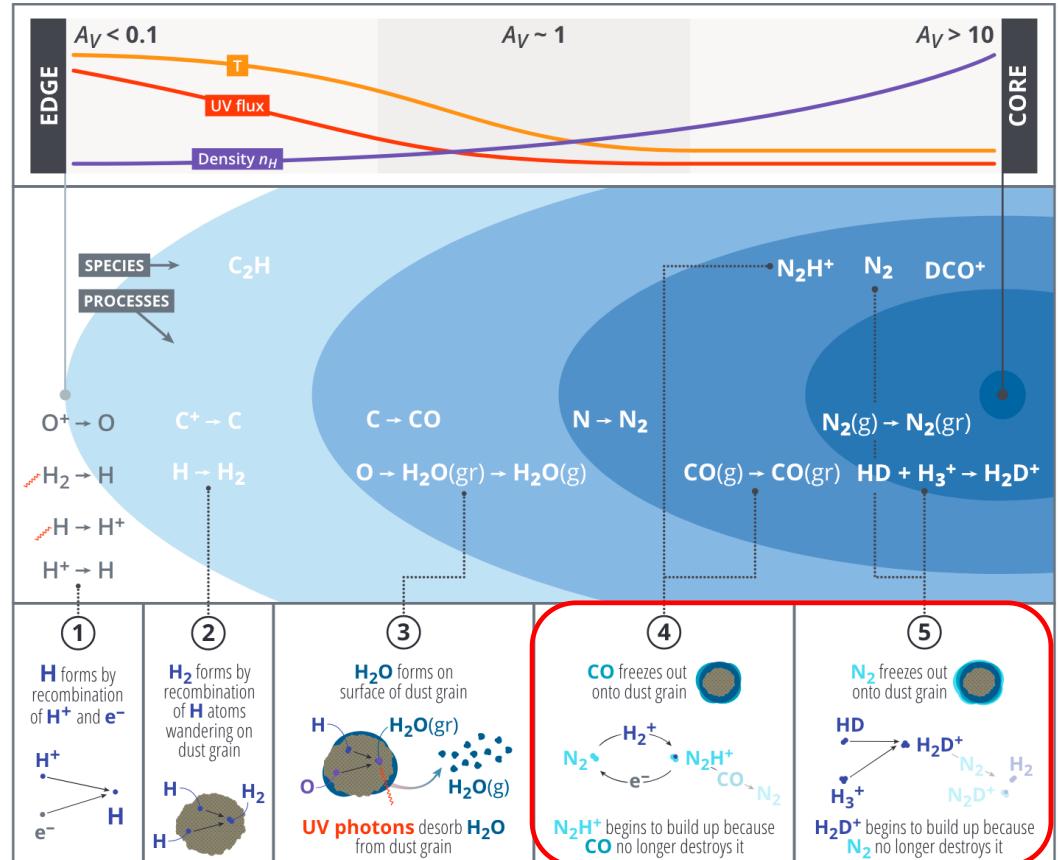
Benefits of observing Isotopes:

- \*Chemical ‘clocks’ that can age molecular clouds and trace the chemical evolution\*

Big Question in Astrochemistry:

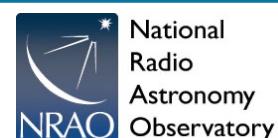
**How much of the material formed early on in the molecular cloud gets inherited to the next stages of star and planet formation?**

*Isotopes help us answer this question!*



Oberg & Bergin 2021

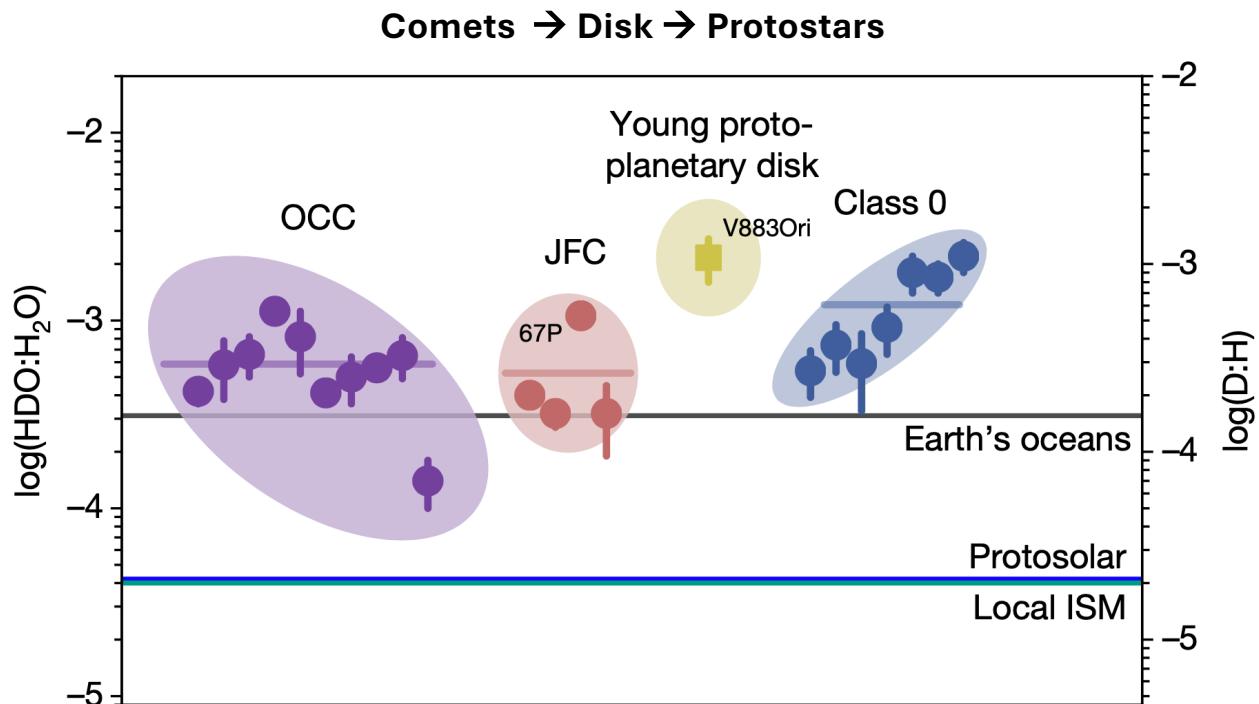
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## Isotopologues (ERA 7.7)

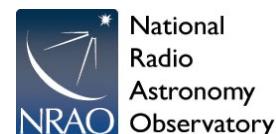
HDO:H<sub>2</sub>O ratio does not strongly evolve from the protostar phase to the disk!

Limited reprocessing of material from early star formation to solar system bodies

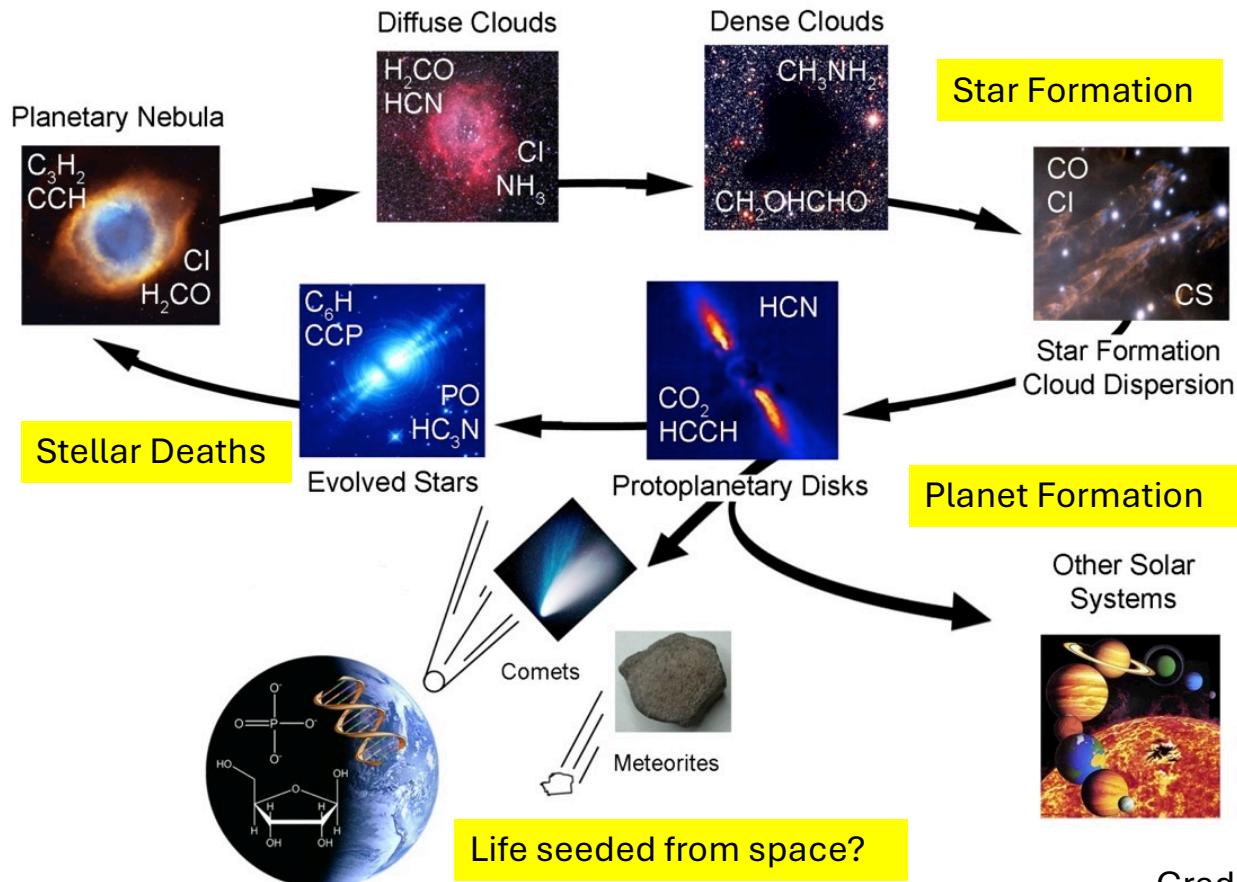
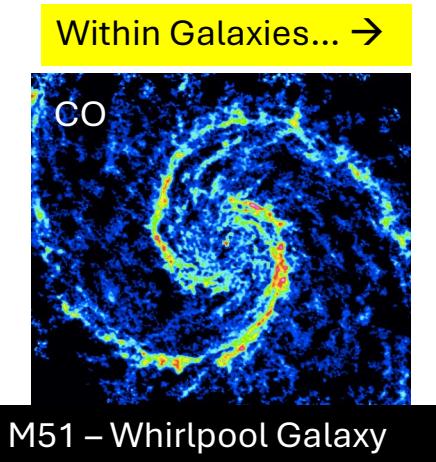


Tobin 2023, Nature

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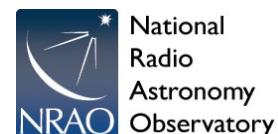


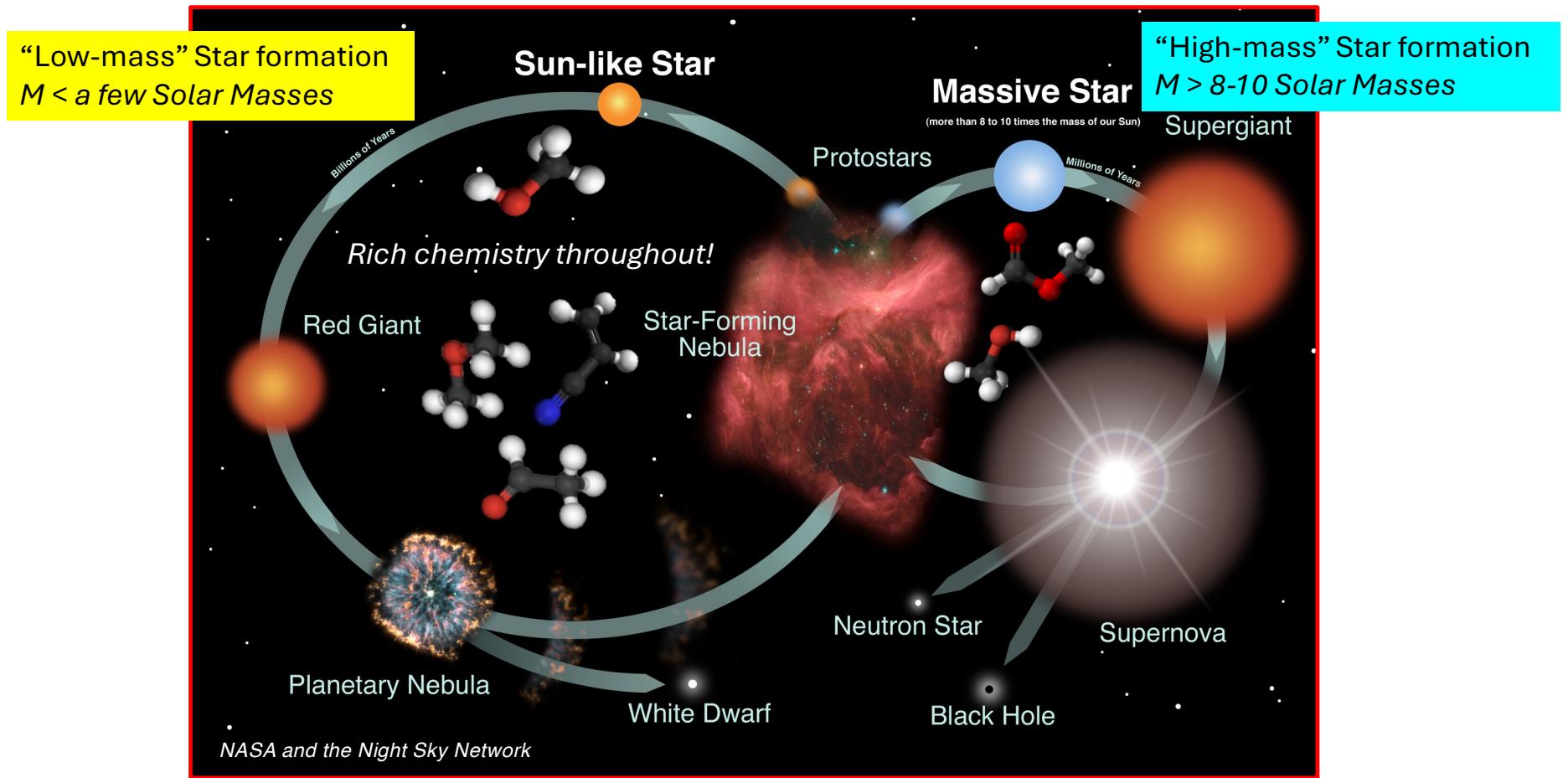
# Molecular Life Cycle



Credit: L. Ziurys

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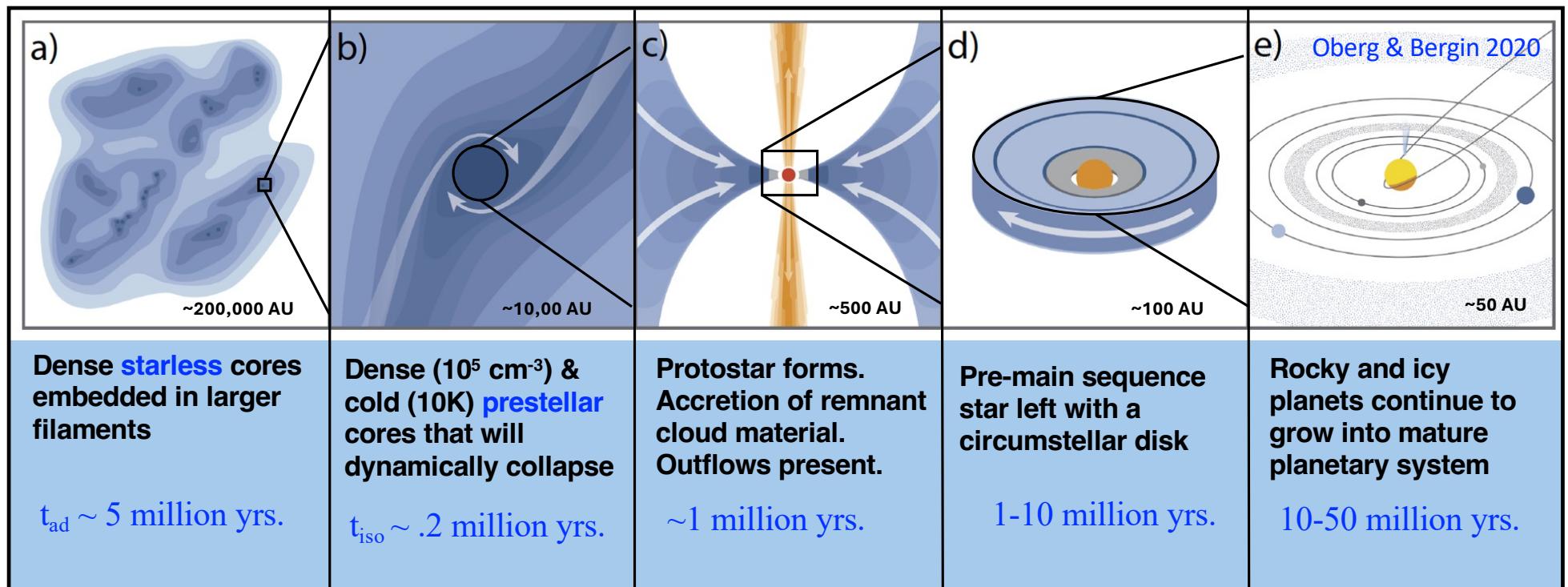




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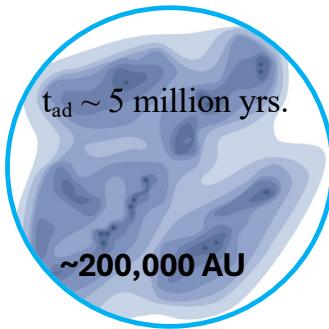


## Low-mass ( $M \leq$ a few $M_{\odot}$ ) Star Formation



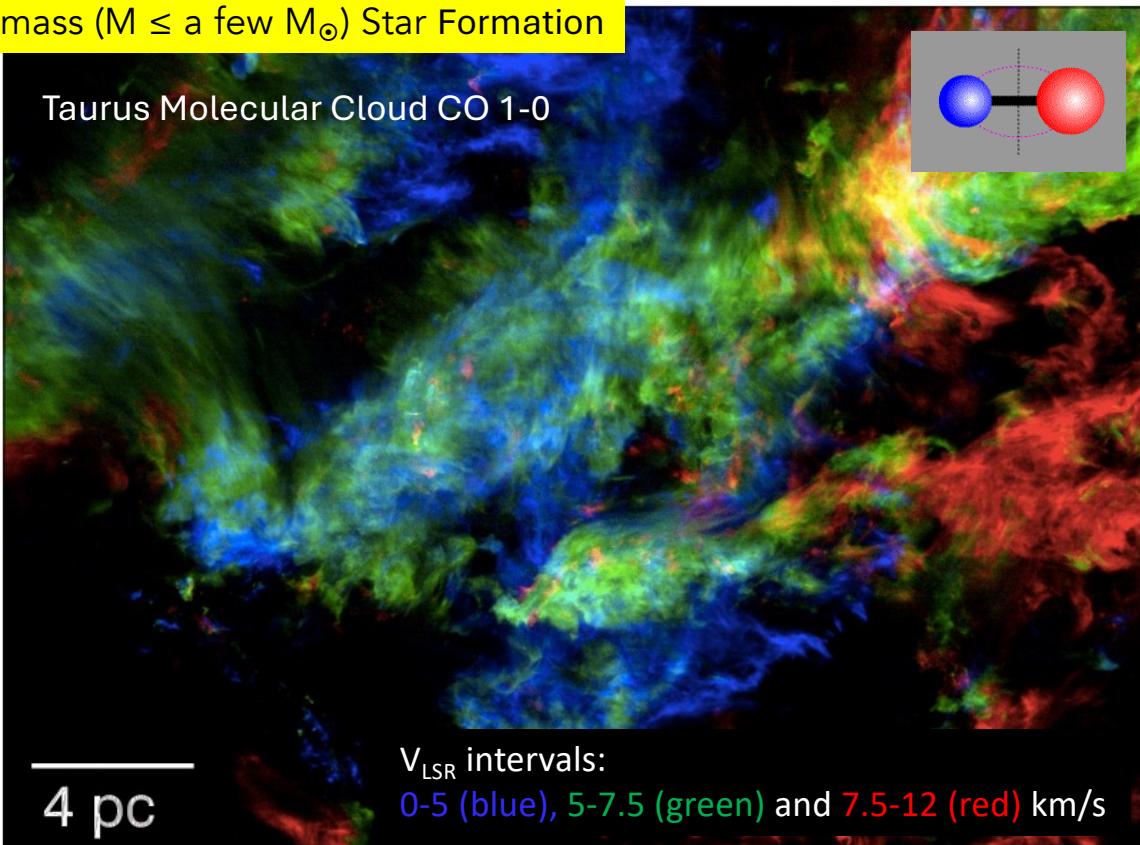
## Molecular Line Data

Molecular clouds are comprised of molecular gas (mostly H<sub>2</sub> and CO) and dust which form filamentary structures

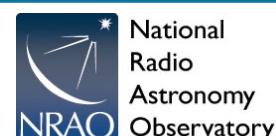


Low-mass ( $M \leq$  a few  $M_\odot$ ) Star Formation

Taurus Molecular Cloud CO 1-0

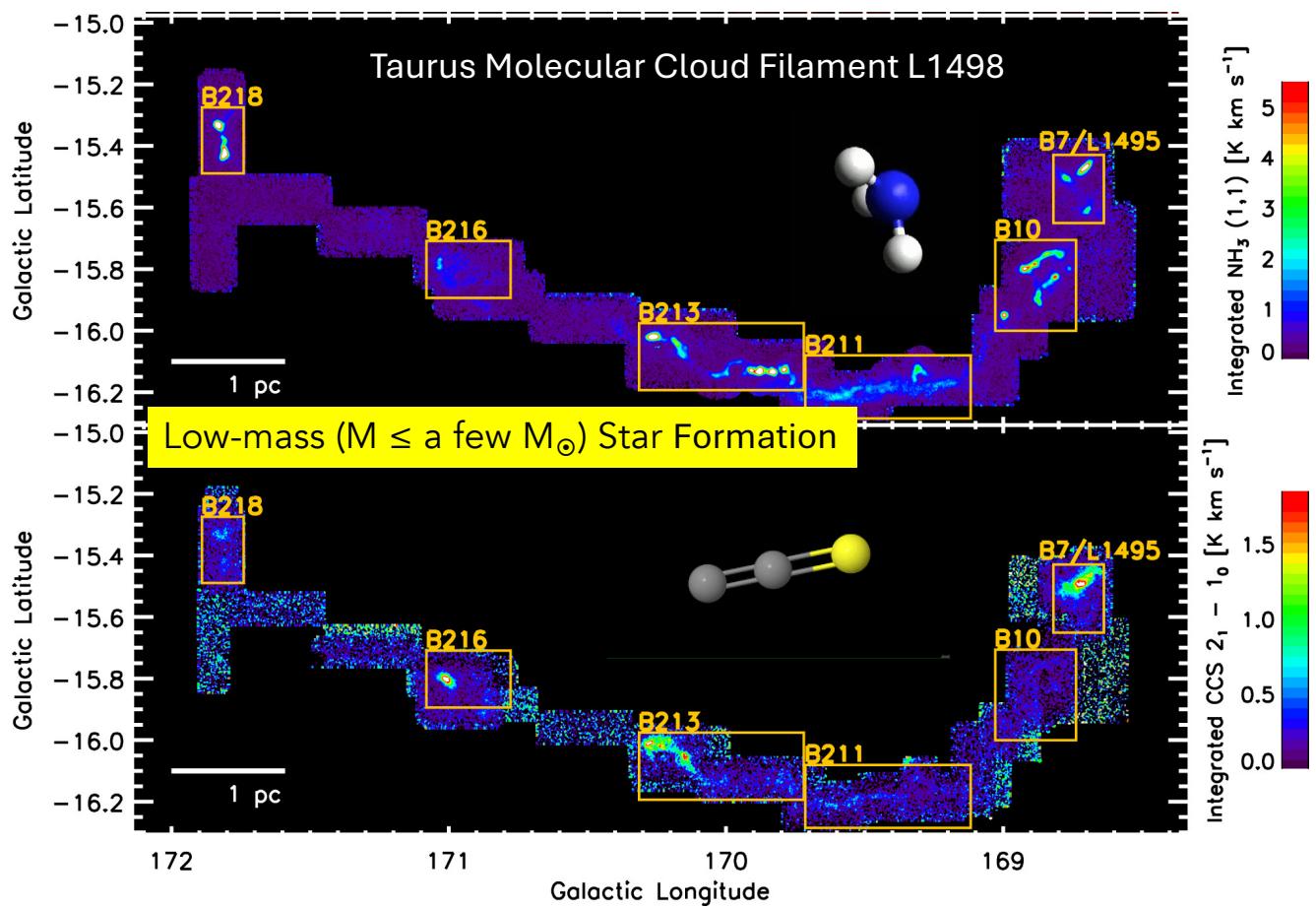
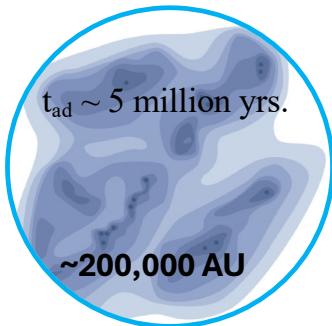


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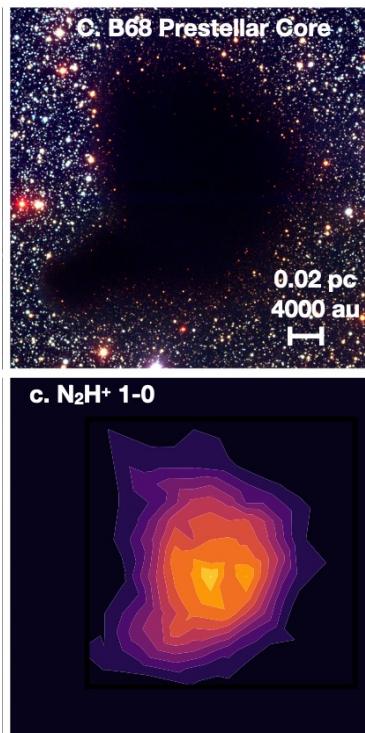
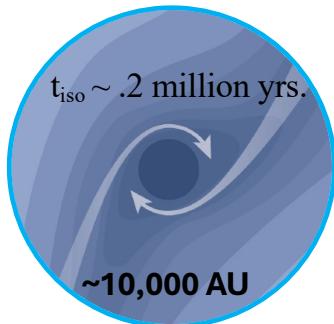
## Molecular Line Data

The filamentary structures are also traced by more 'exotic' molecular species, such as  $\text{NH}_3$  and CCS



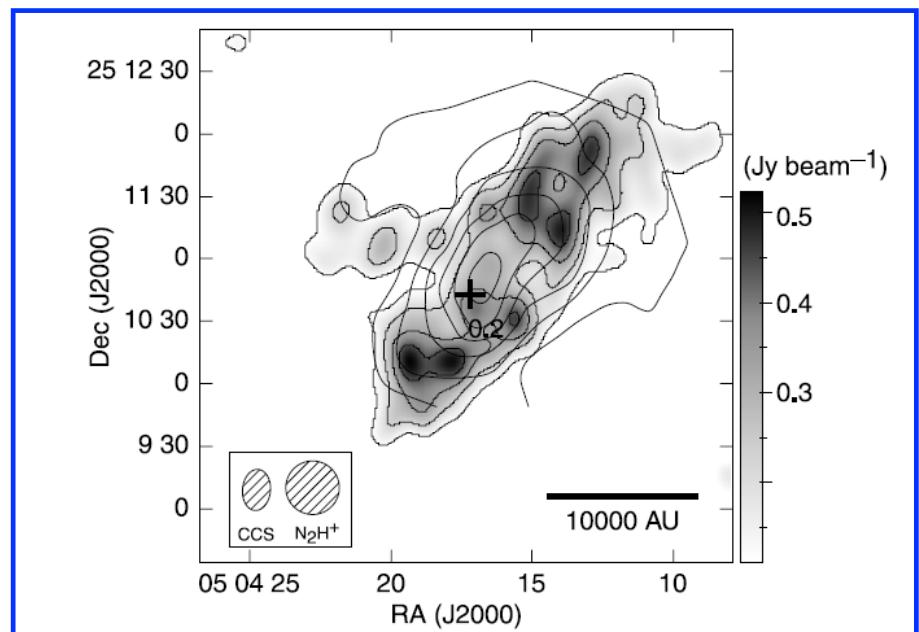
## Molecular Line Data

Dense ( $10^5 \text{ cm}^{-3}$ ) & cold (10K) *starless* and dynamically evolved  *prestellar* cores collapse due to gravity and external cloud pressure



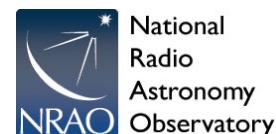
Oberg & Bergin 2020

CCS (greyscale) → freeze out towards denser and colder center  
N<sub>2</sub>H<sup>+</sup> (contours) → traces high densities in and around core



\*Molecules are powerful probes of the physical conditions!

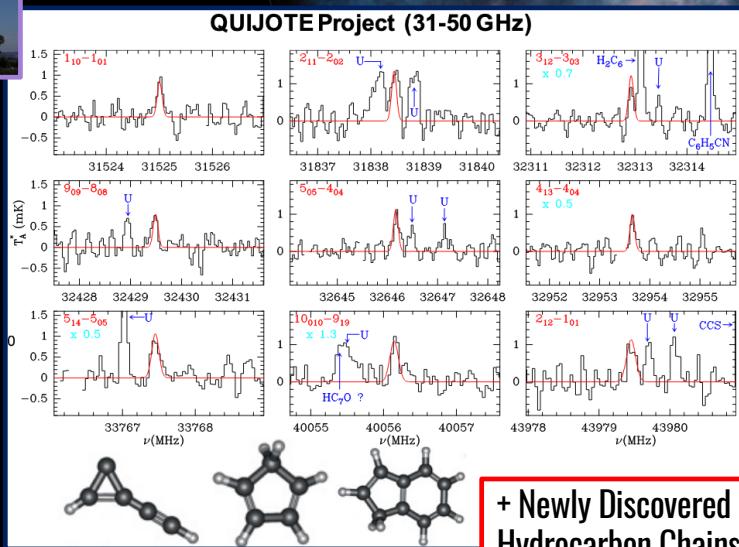
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**Sensitive, unbiased line surveys are ongoing and continually finding new molecules in the dense cloud TMC-1!**

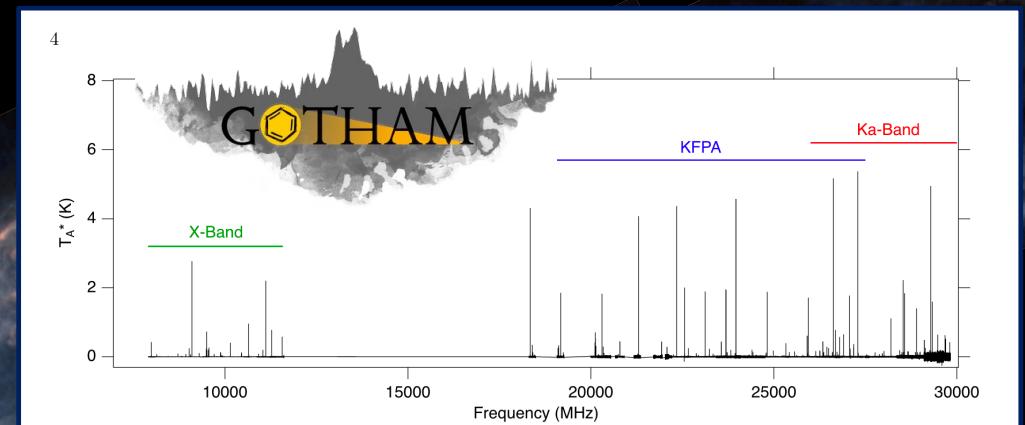


Yebes  
Dish



Cernicharo et al., 2021 & QUIJOTE team

+ Newly Discovered Hydrocarbon Chains and Cycles



McGuire et al. 2018, 2020



GBT 100m Dish

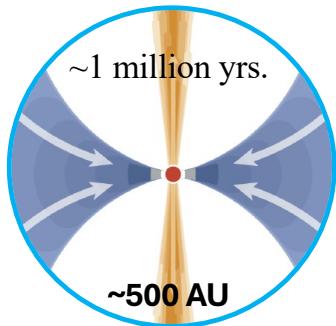


First Aromatic Hydrocarbon, Benzonitrile!

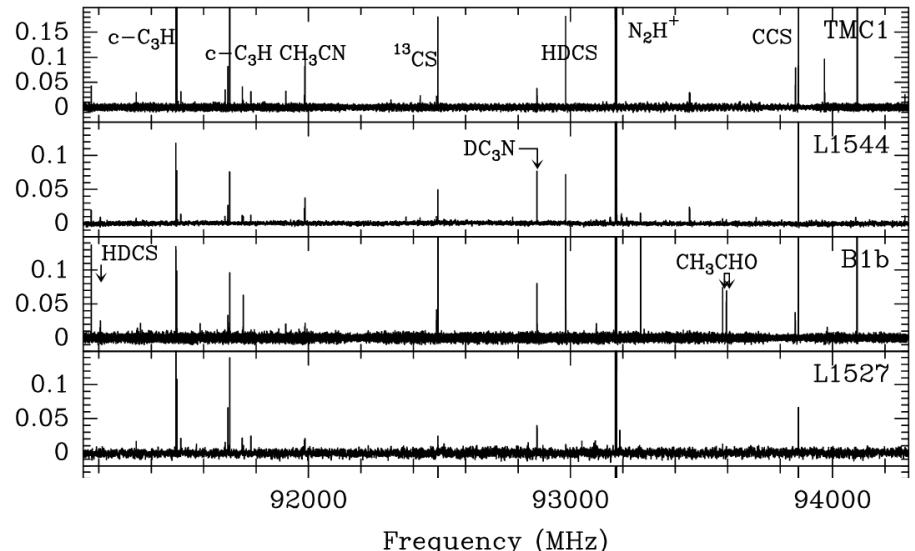
Blue 160μm, Green 250+350 μm, Red 500 μm  
Credit: Herschel Gould Belt Team

## Molecular Line Data

A *protostar* forms.  
Accretion of remnant  
cloud material.  
Outflows and jets are  
present.

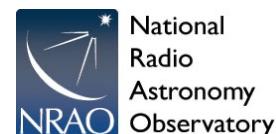


Low-mass ( $M \leq$  a few  $M_{\odot}$ ) Star Formation



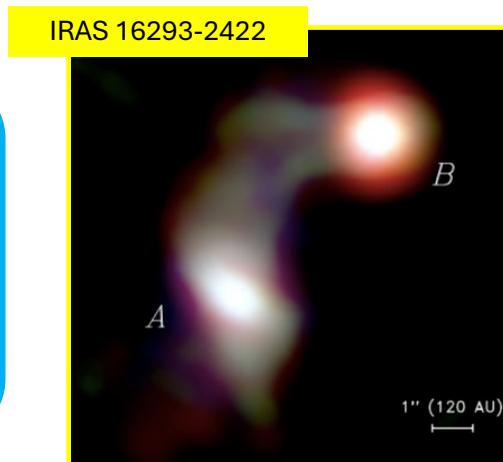
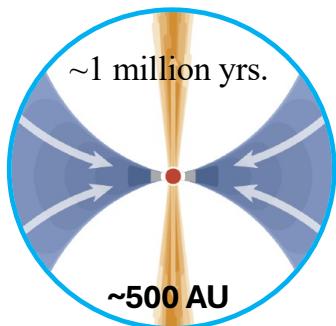
Lefloch et al., 2018

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## Molecular Line Data

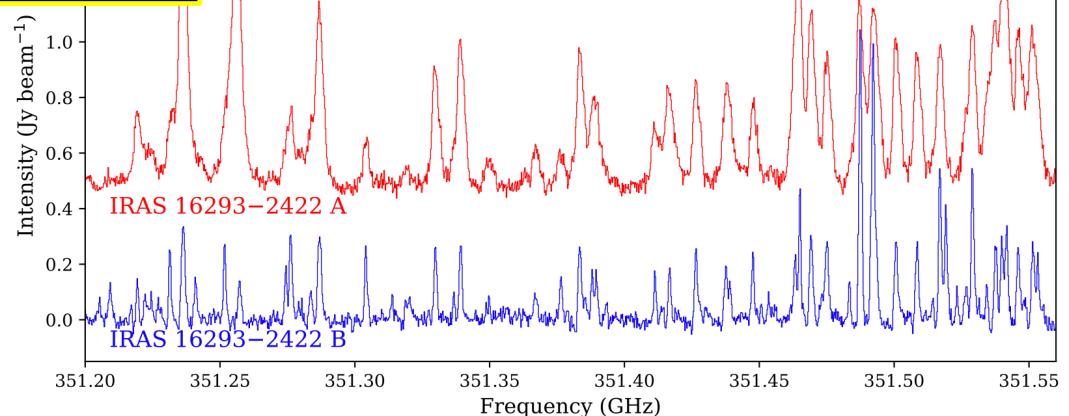
A *protostar* forms.  
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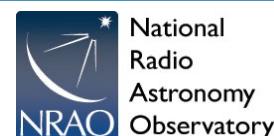
Low-mass ( $M \leq$  a few  $M_{\odot}$ ) Star Formation

Large program targeting many lines: ALMA PILS

Manigand et al., 2020

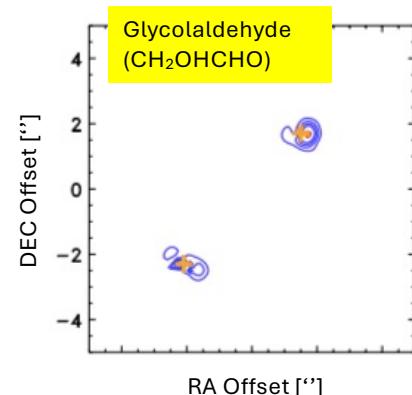
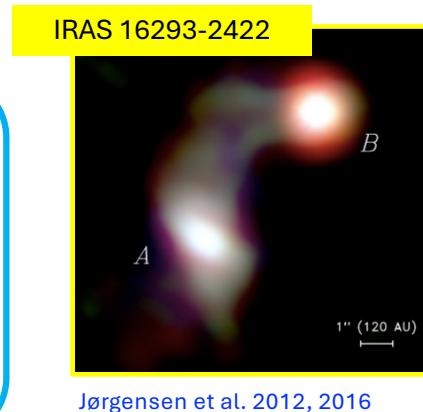
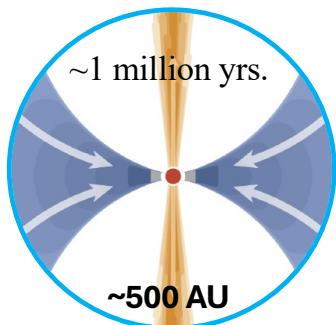


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## Molecular Line Data

A *protostar* forms.  
Accretion of remnant  
cloud material.  
Outflows and jets are  
present.

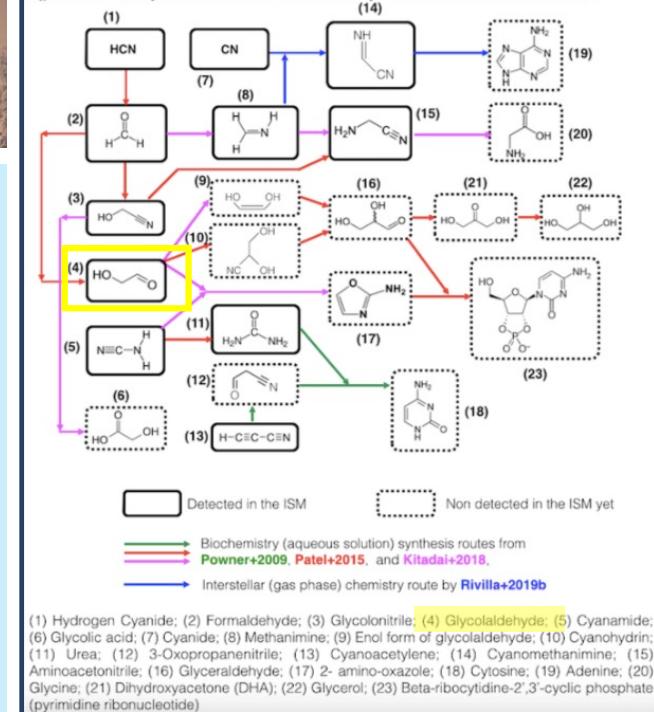


Life appeared on Earth about 4 billion years ago, but we do not know the processes that made it possible.

One of the proposed scenarios is the so-called **ribonucleic acid RNA-world**, which suggests that early forms of life relied solely on (RNA) to store genetic information and to catalyze chemical reactions.

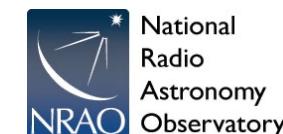
## Low-mass ( $M \leq$ a few $M_{\odot}$ ) Star Formation

Figure 1. Summary of the chemical scheme of the primordial RNA-world scenario.

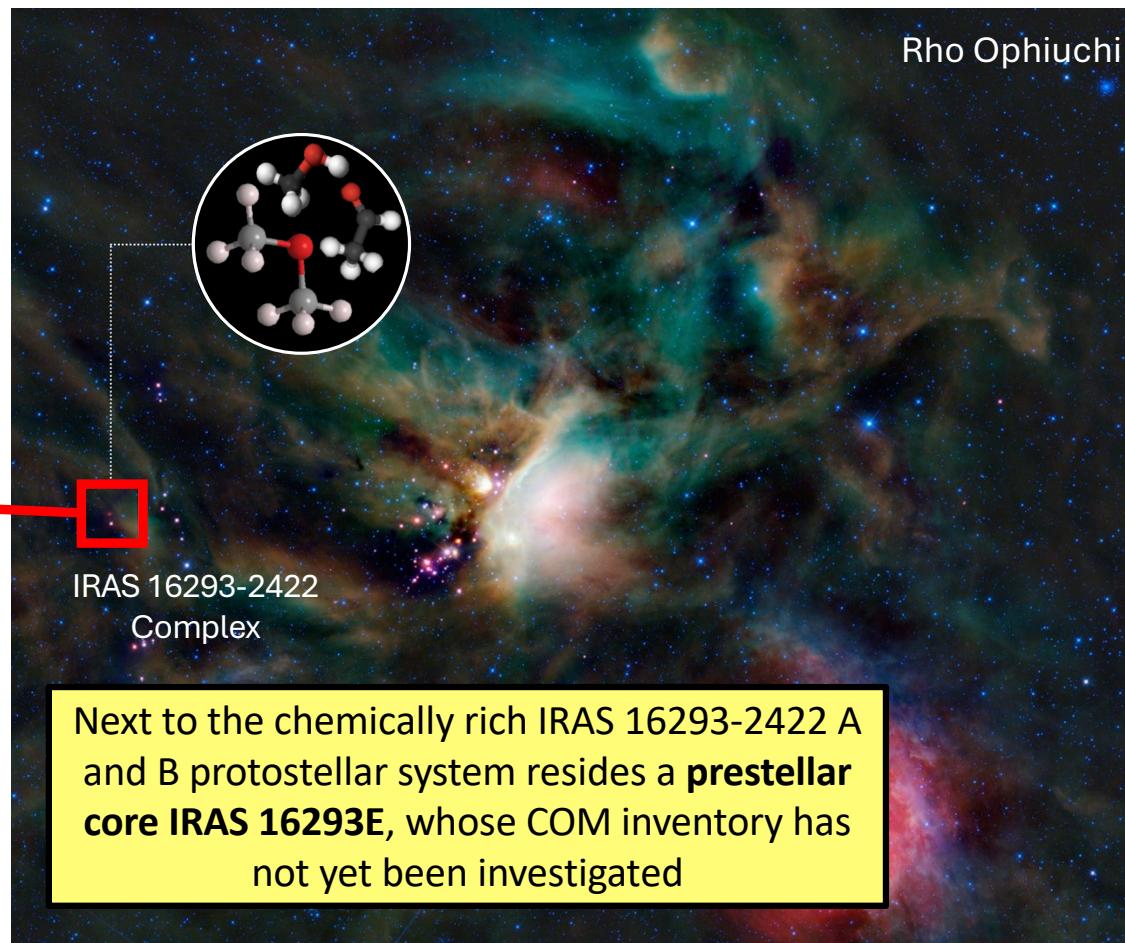
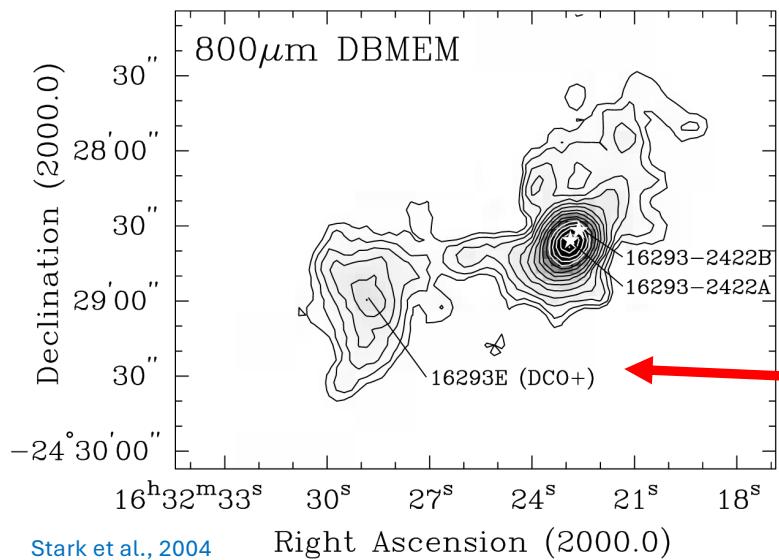


Jimenez-Serra et al. 2020

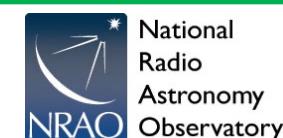
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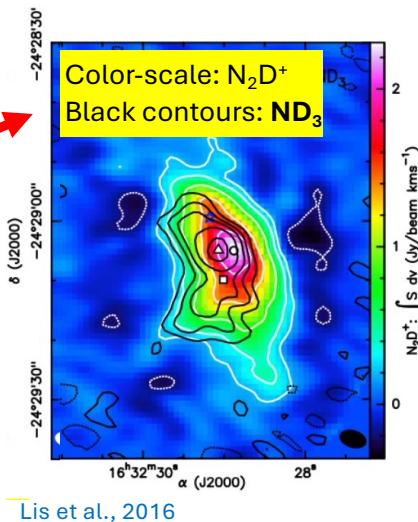
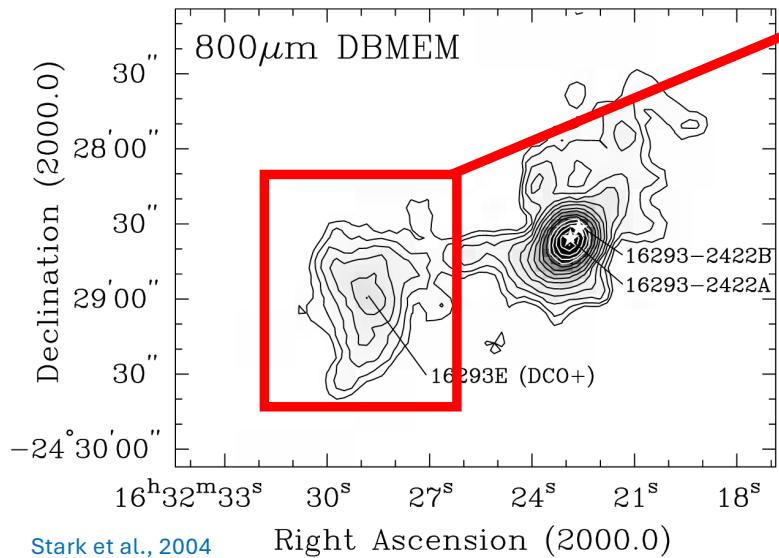
# IRAS 16293E



Fractionation II, Florence, Italy, Nov 4<sup>th</sup>- 7<sup>th</sup>, 2024  
Contact: sscibell@nrao.edu



# IRAS 16293E

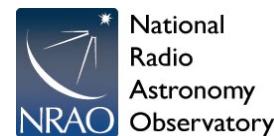


Additionally, IRAS 16293 A, B and E all show some of the **highest levels of deuteration** in the ISM!

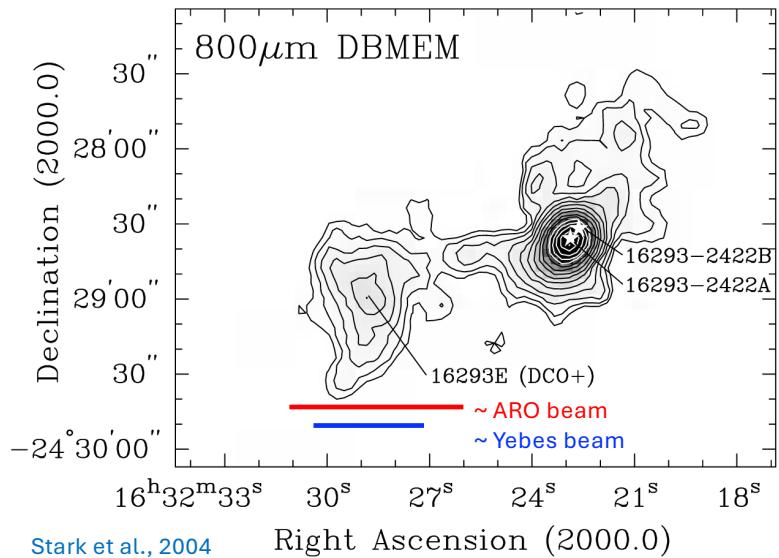
- **Deuterated COMs (dCOMs)** in particular provide an **exciting probe into chemical histories**, as high deuteration levels in protostellar systems (e.g., IRAS16293 A and B with 2-8% and D<sub>2</sub>/D  $\sim$  20%) compared to typical values in the ISM (D/H  $\sim$  10<sup>-5</sup>) suggest **COMs are forming during the time deuteration is enhanced – in cold (10 K) prestellar cores!**
- To date, only a handful (< 3) of prestellar cores have had detections of both singly- and doubly-deuterated versions of the simplest COM – methanol (Lin et al., 2023)

**IRAS16292E is a prime target to search for COMs and dCOMs!**

Fractionation II, Florence, Italy, Nov 4<sup>th</sup>- 7<sup>th</sup>, 2024  
Contact: sscibell@nrao.edu

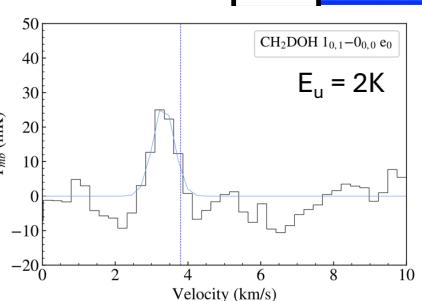
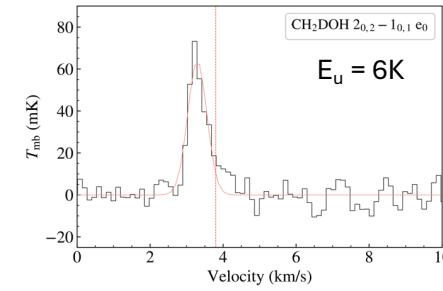


# IRAS 16293E

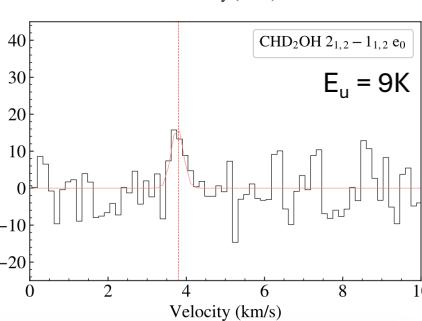
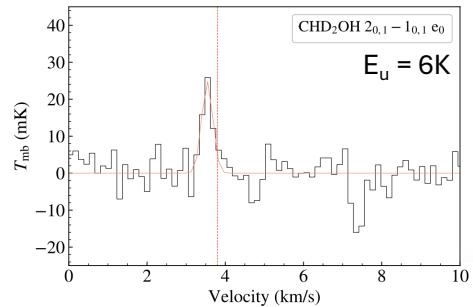


Single-pointed observations w/

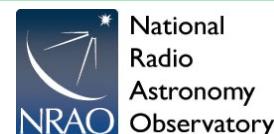
Singly Deuterated Methanol!



Doubly Deuterated Methanol!



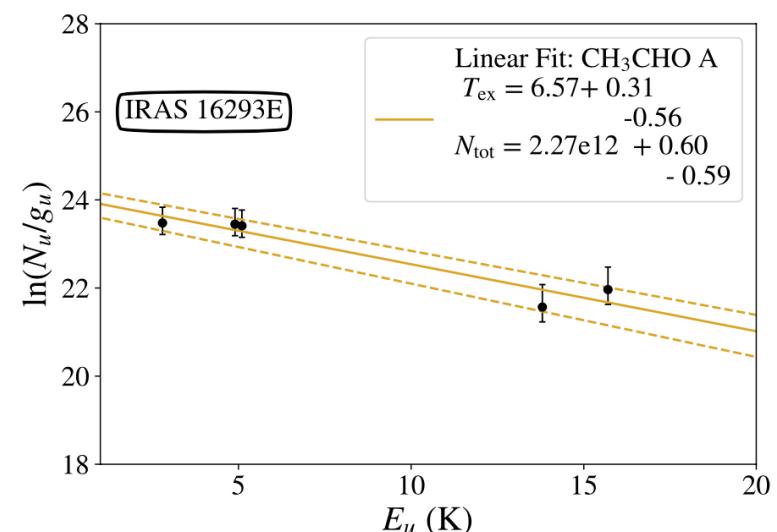
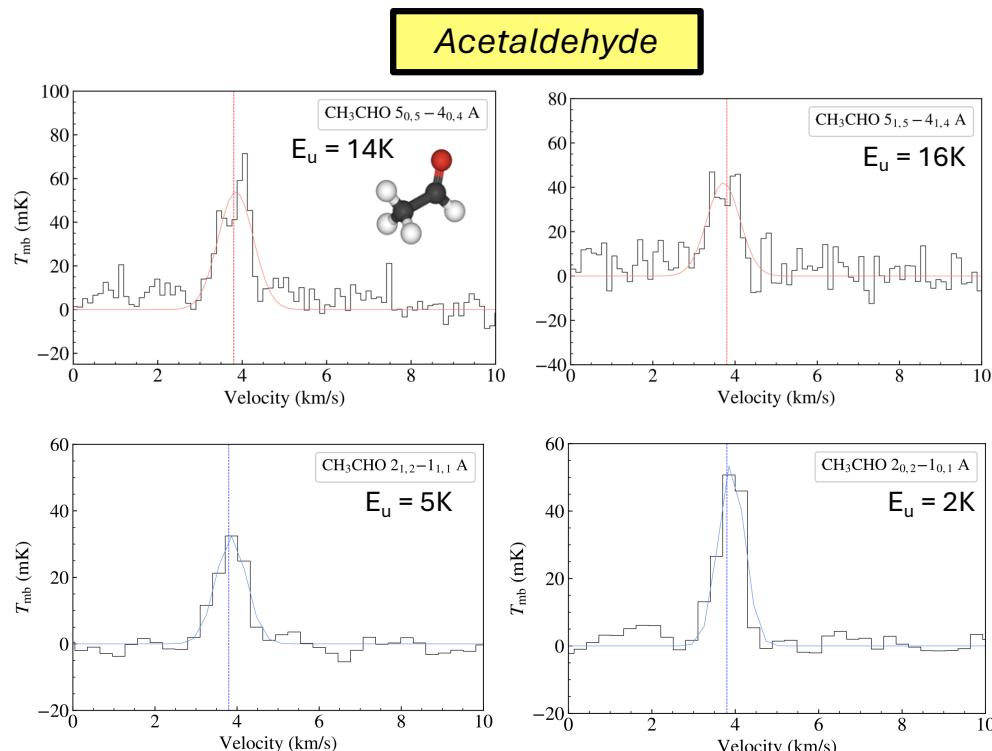
Fractionation II, Florence, Italy, Nov 4<sup>th</sup>- 7<sup>th</sup>, 2024  
Contact: sscibelli@nrao.edu



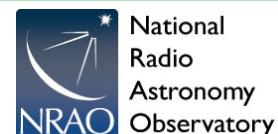
Scibelli et al., in prep

# IRAS 16293E

*COM and dCOM column densities and excitation temperatures*



Fractionation II, Florence, Italy, Nov 4<sup>th</sup>- 7<sup>th</sup>, 2024  
Contact: sscibell@nrao.edu

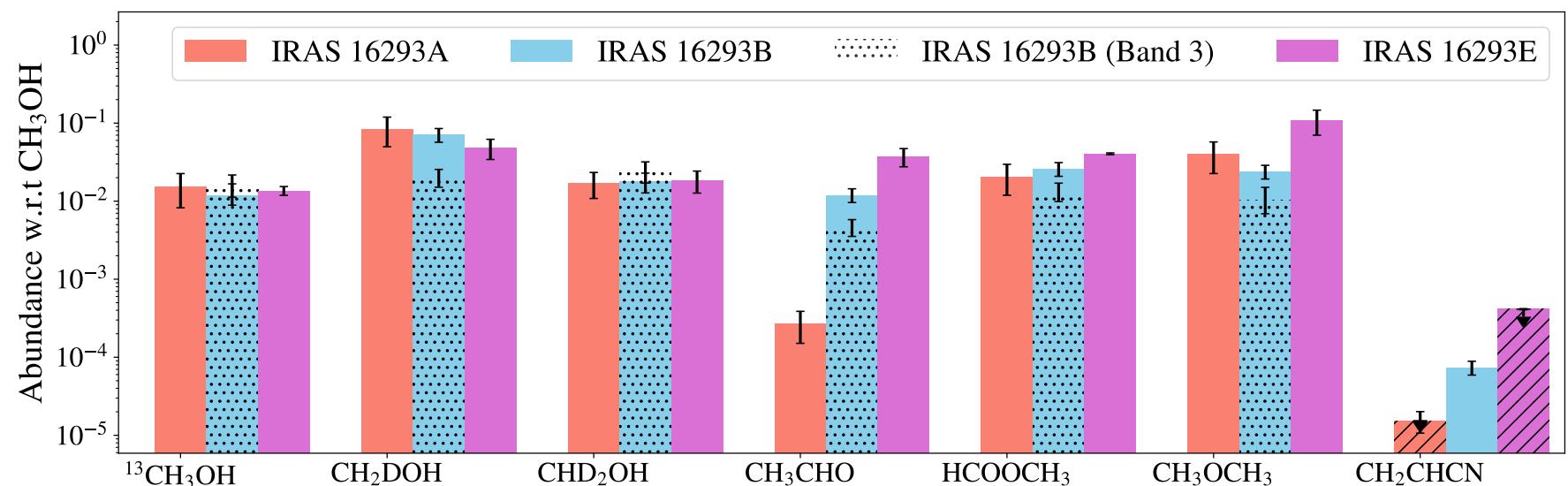


Scibelli et al., in prep

# IRAS 16293E

Striking similarity in abundances in IRAS 1293 A, B and E!  
In particular, CHD<sub>2</sub>OH shows the best agreement

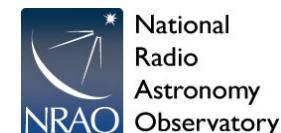
The enhanced deuterated methanol in protostars IRAS 16293 A and B was set during the prestellar phase!



Including data from: Jørgensen et al. 2018; Calcutt et al. 2018; Manigand et al. 2020; Drozdovskaya et al. 2022, Nazari et al. (2024)

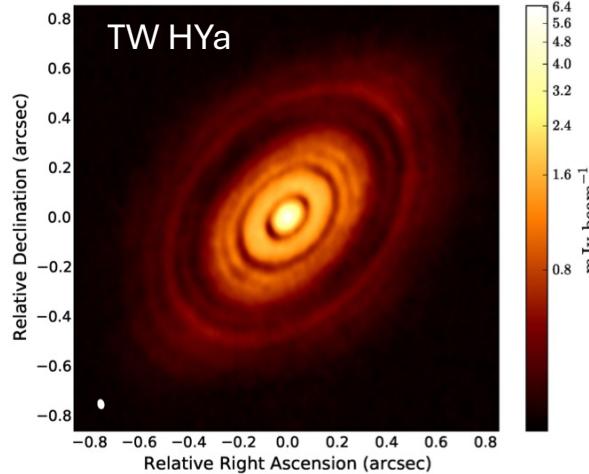
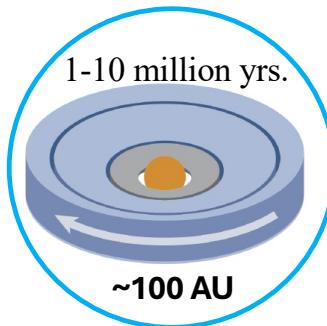
Scibelli et al., in prep

Fractionation II, Florence, Italy, Nov 4<sup>th</sup>- 7<sup>th</sup>, 2024  
Contact: sscibell@nrao.edu



## Molecular Line Data

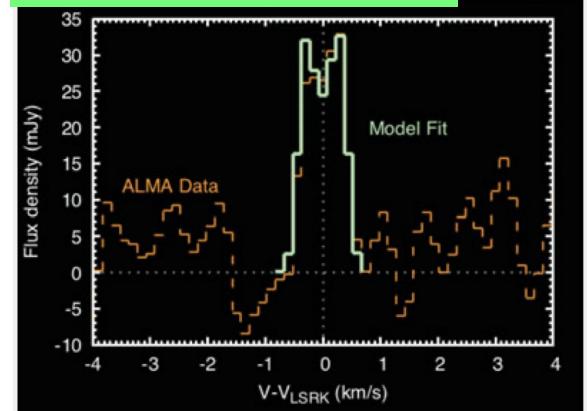
A *protoplanetary disk* show gaps in rings that signify planet formation!



Low-mass ( $M \leq$  a few  $M_{\odot}$ ) Star Formation

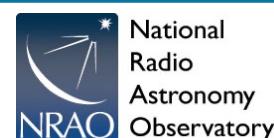
Challenging to observe COMs in such small objects, need sensitive telescopes!

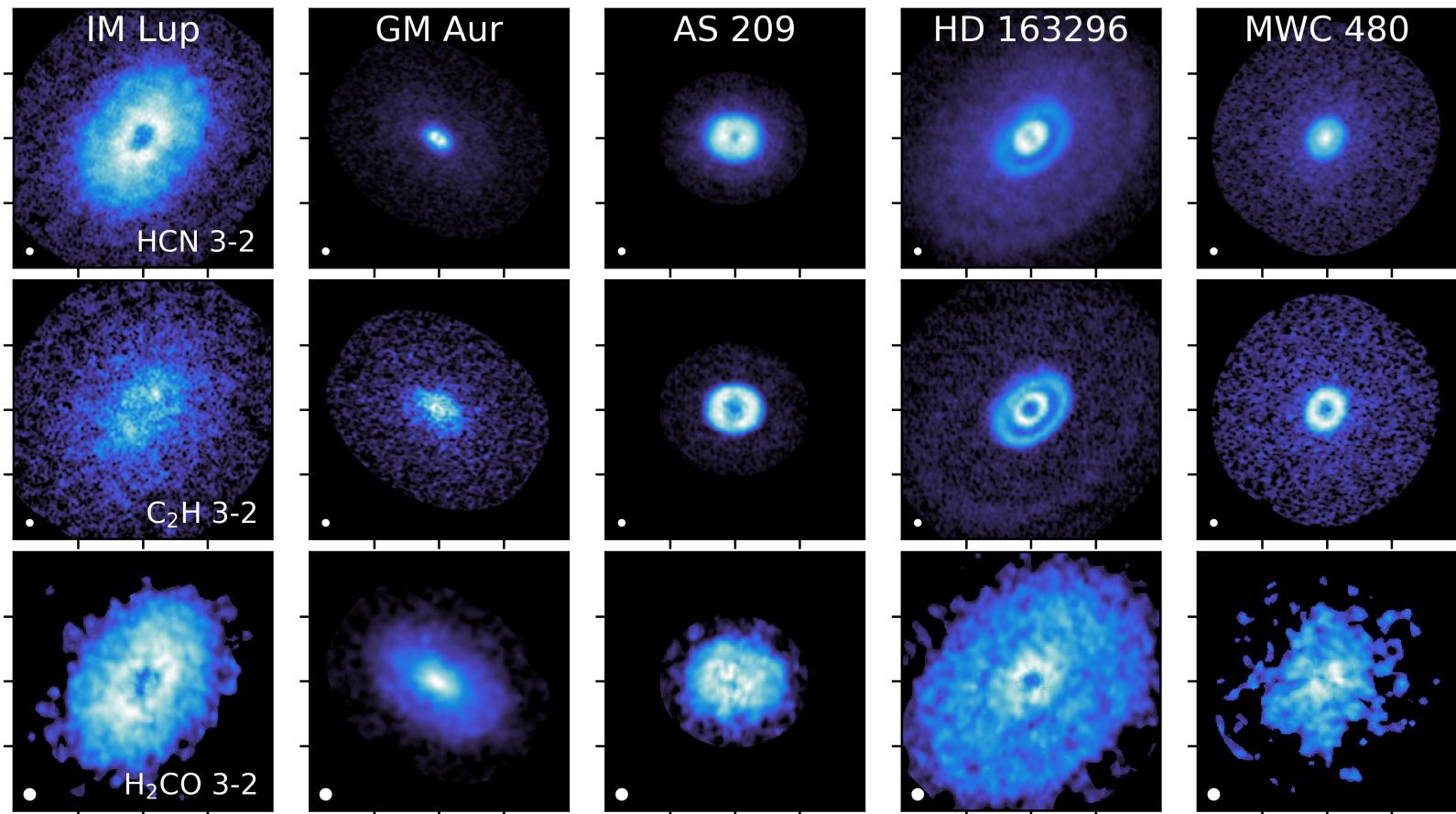
Methanol,  $\text{CH}_3\text{OH}$ , line profile



Walsh et al. 2016, 2017

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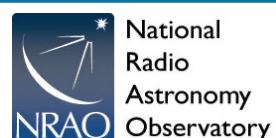


**MAPS  
Large Program**

Disk structure is even seen in molecular emission!

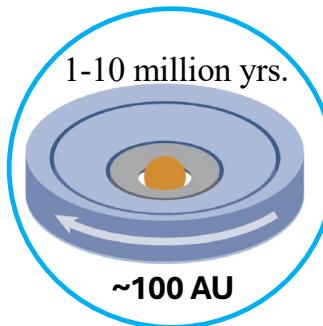
Oberg et al., 2021

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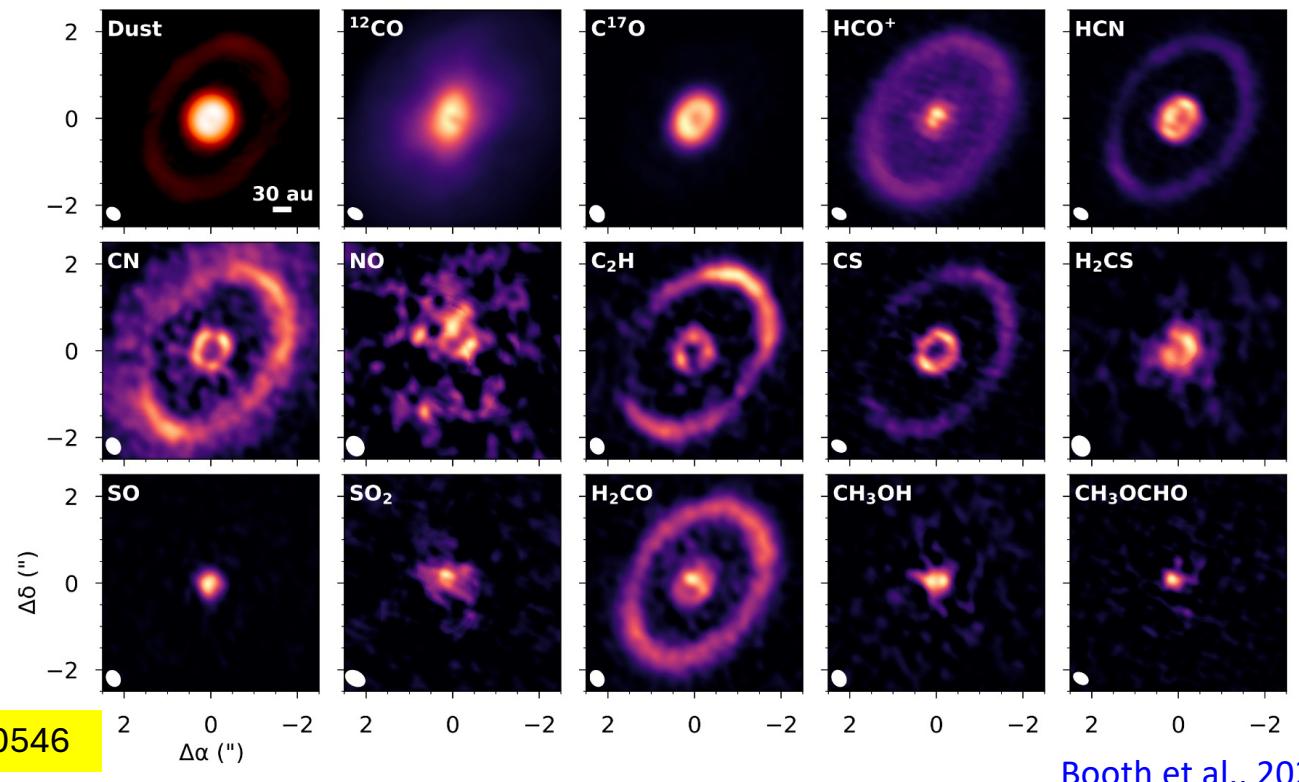
## Molecular Line Data

A *protoplanetary disk* show gaps in rings that signify planet formation!



HD 100546

Larger COMs now seen in disks around more massive A and B stars!



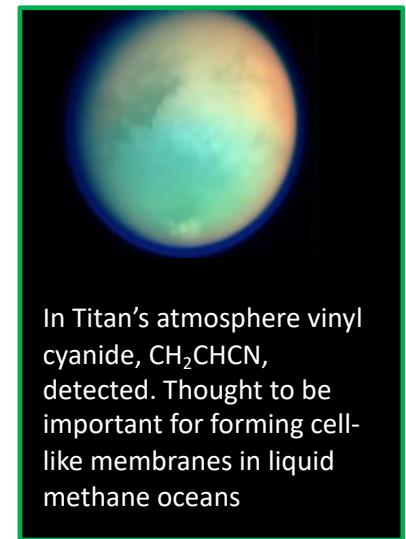
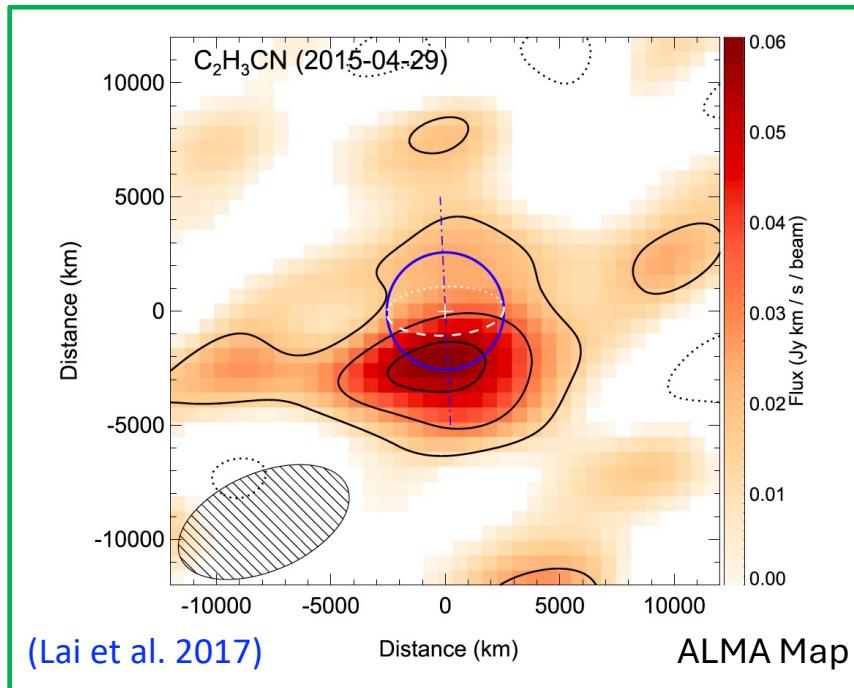
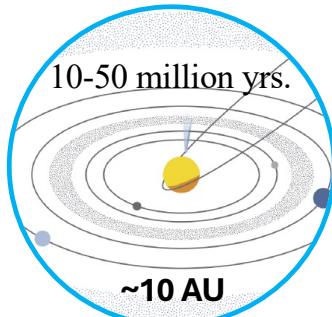
Booth et al., 2024a

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## Molecular Line Data

Rocky and icy planets and moons, as well as planetesimals (e.g., asteroids, comets), continue to grow into a mature *planetary system*

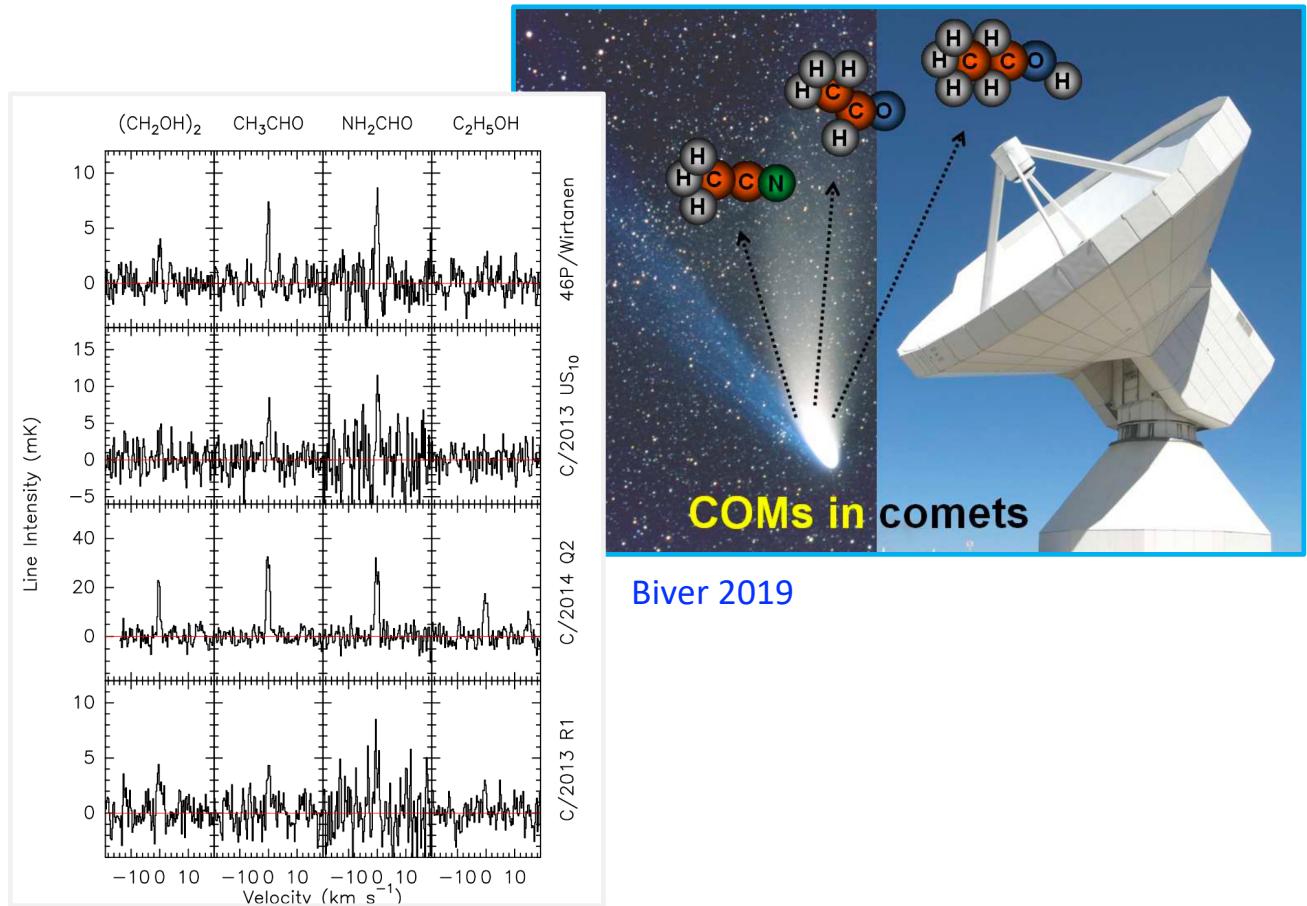
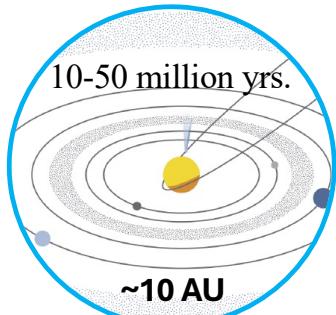


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## Molecular Line Data

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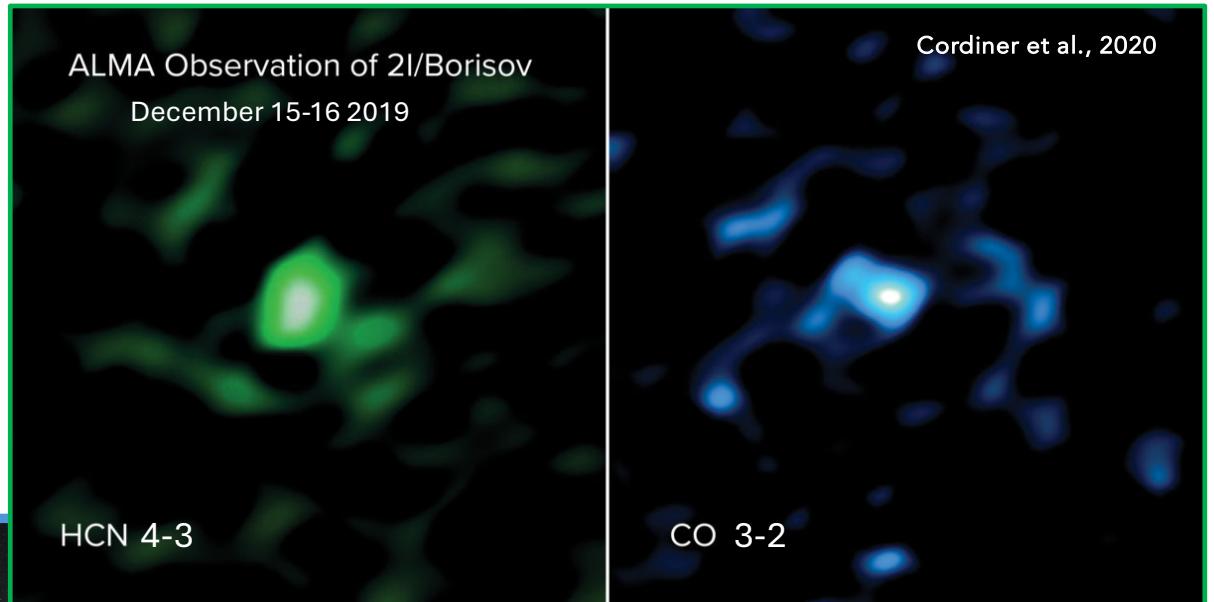


## Molecular Line Data

- The first confirmed [interstellar](#) comet!
- The [HCN](#) abundance similar to that of comets in our Solar System
- The [CO](#) abundance is among the highest observed in any comet within 2 au of the Sun!
- 2I/Borisov must have formed in a relatively CO-rich environment in the very cold, outer regions of a distant protoplanetary accretion disk (similar to our proto-Kuiper belt)

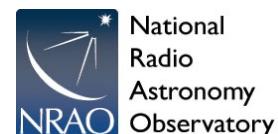


ALMA interferometer



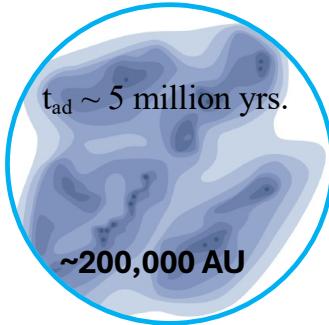
Maps from rotational line spectra

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Contact: [sscibell@nrao.edu](mailto:sscibell@nrao.edu)

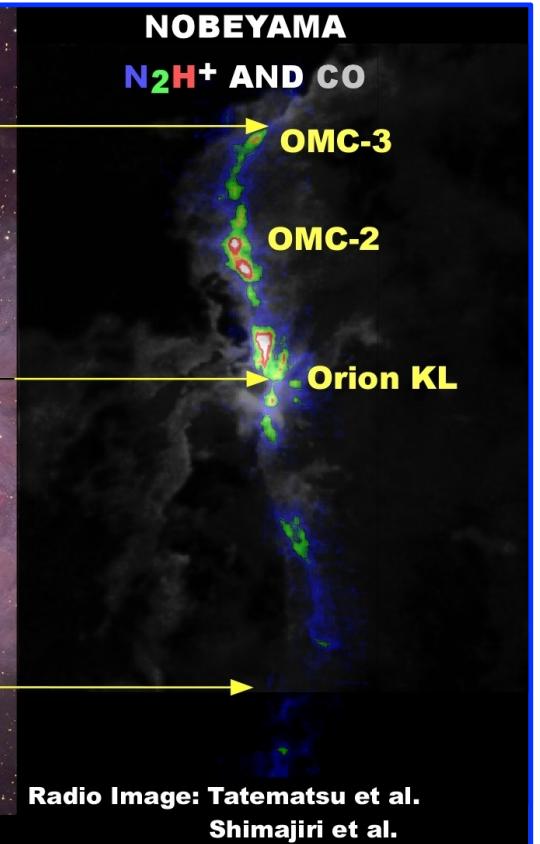
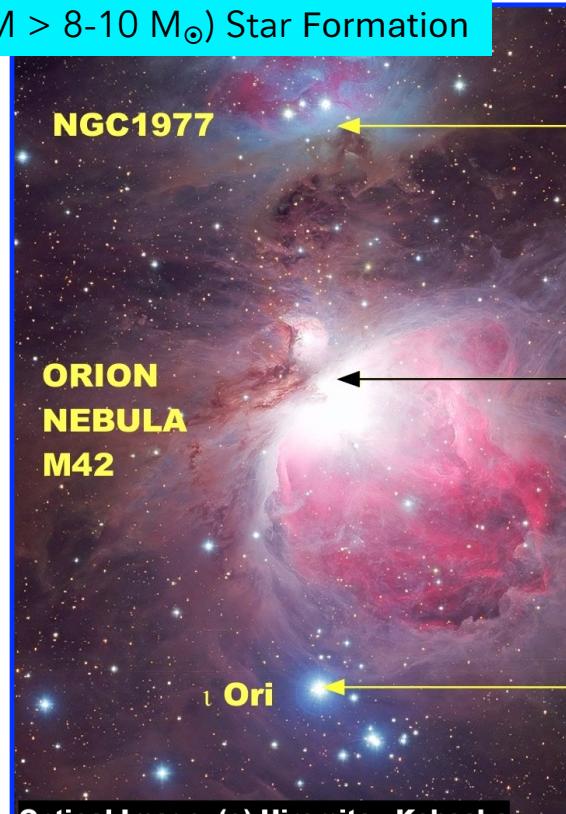


## Molecular Line Data

Molecular clouds are comprised of molecular gas (mostly H<sub>2</sub> and CO) and dust which form filamentary structures



High-mass ( $M > 8-10 M_\odot$ ) Star Formation

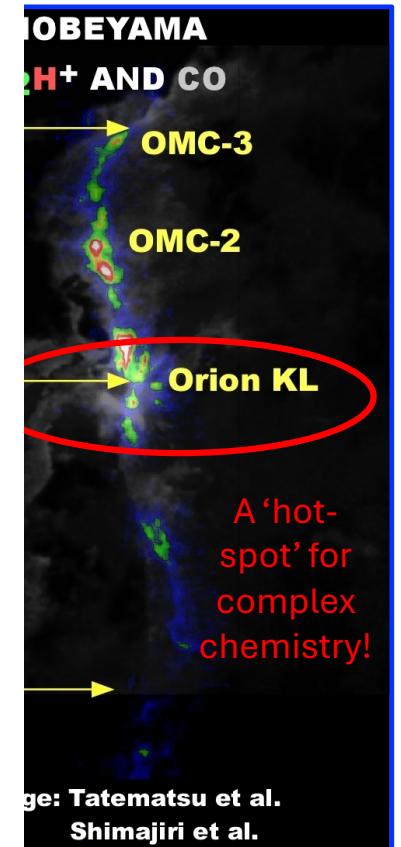
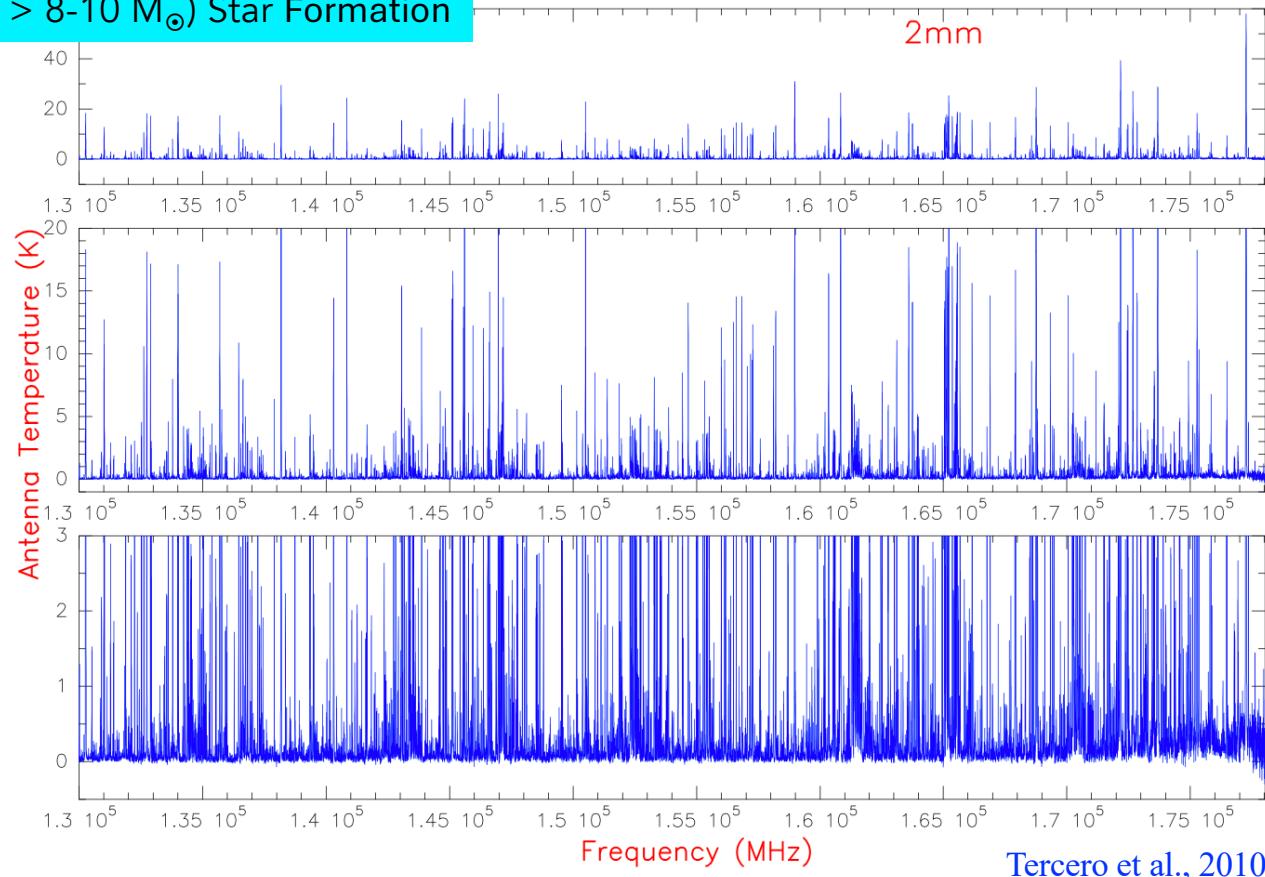


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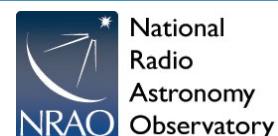


<https://www.nro.nao.ac.jp/~kt/html/kt-e.html>

## High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation

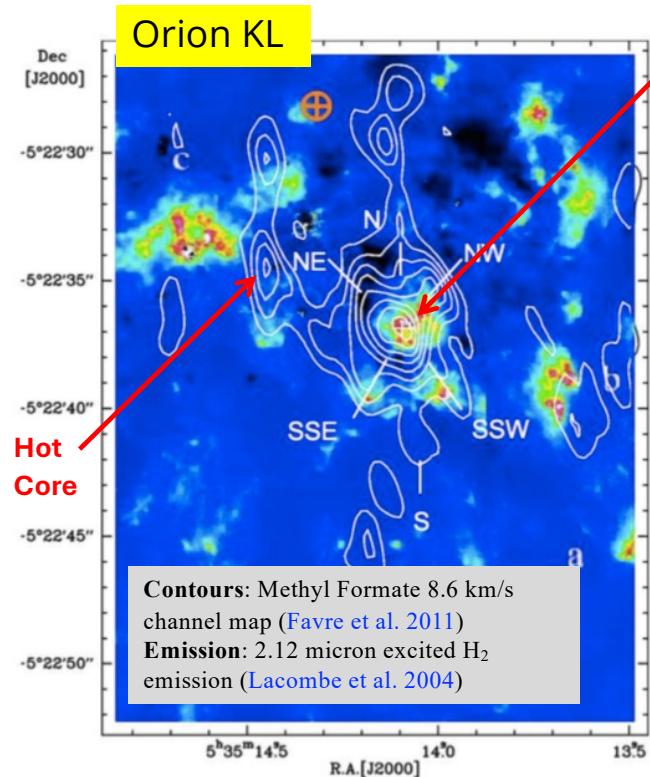


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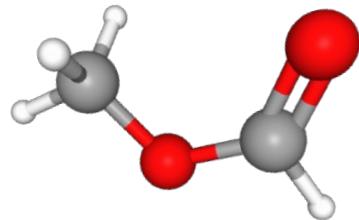


## Molecular Line Data

High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation

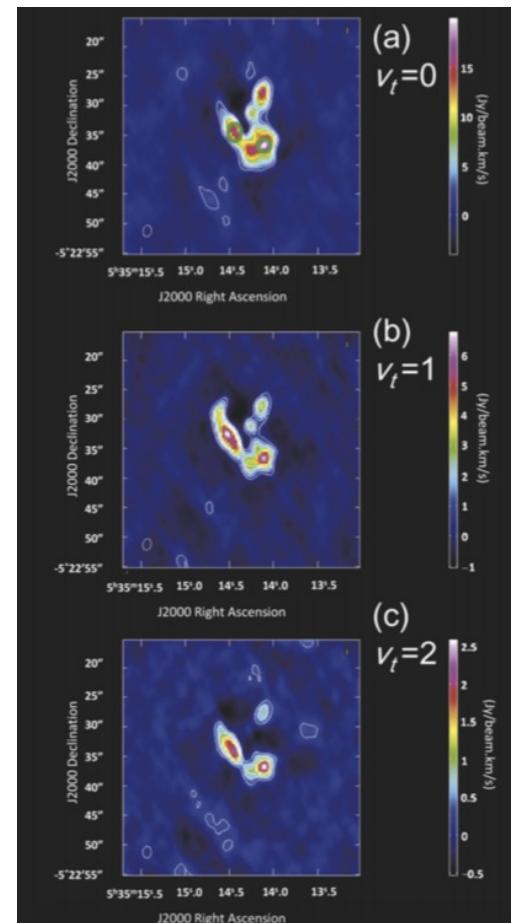


8-atom molecule,  
Methyl Formate,  
 $\text{HCOOCH}_3$ , tracing the  
star-forming ‘hot core’

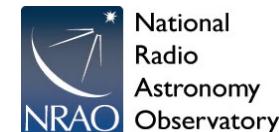


First identification of rotational  
transitions in the second  
vibrationally excited state!

Sakai et al. 2015

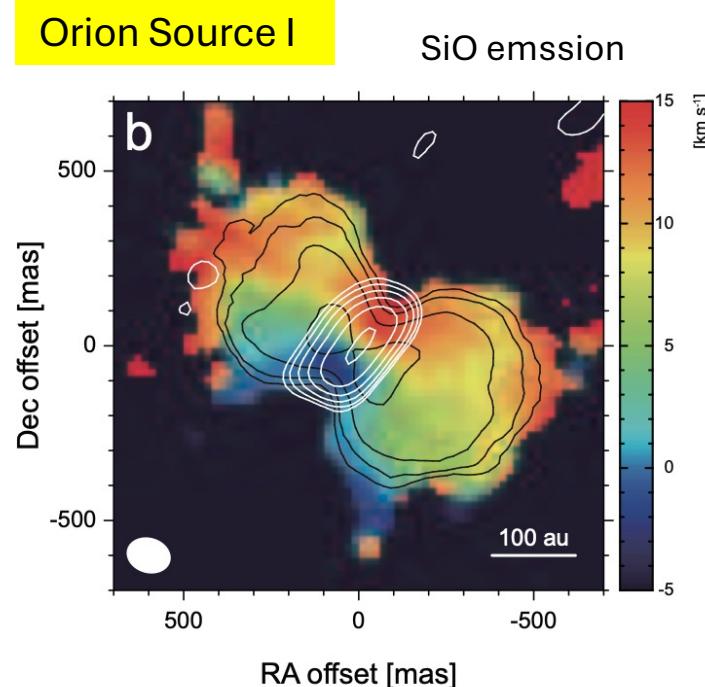


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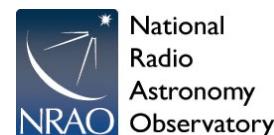
## Molecular Line Data

High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation



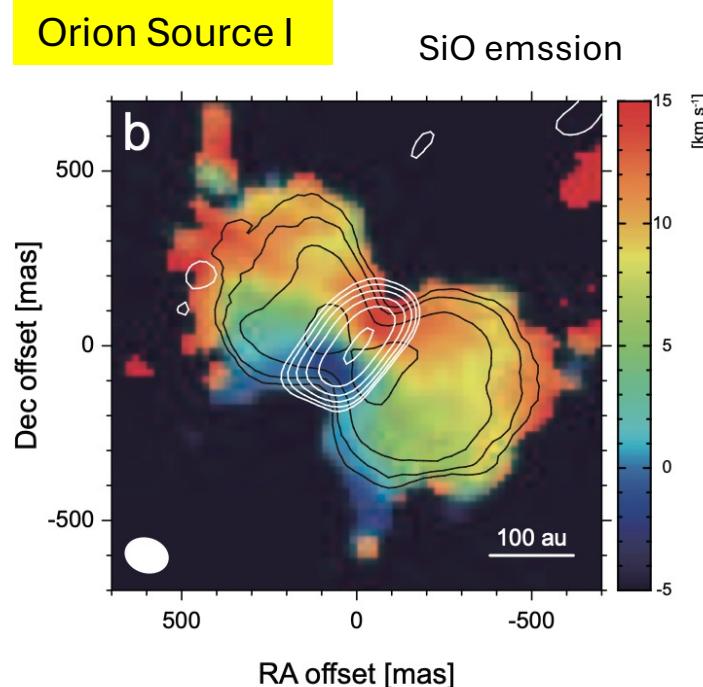
The presence of a **disk-outflow** system (Hirota et al. 2017) indicates that “Orion source I” is accreting, confirming its nature as a young, forming star.

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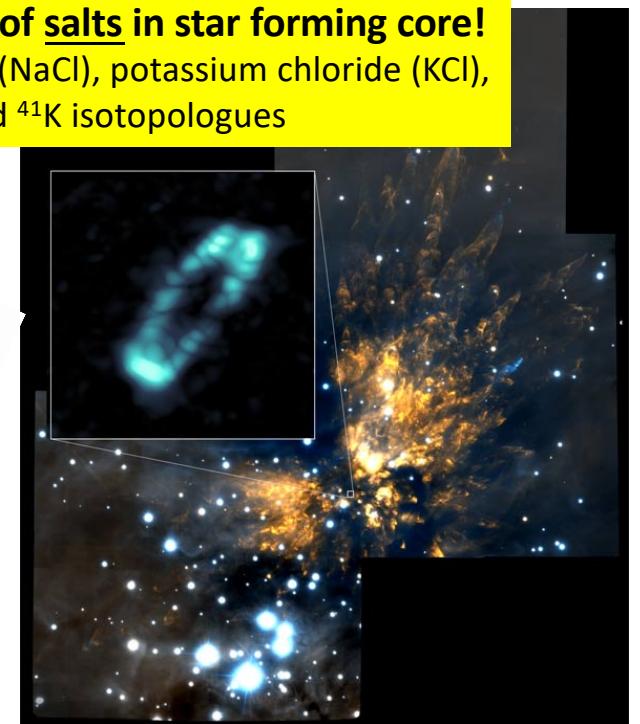
## Molecular Line Data

High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation



**First detection of salts in star forming core!**

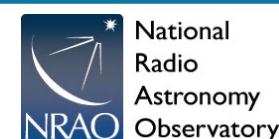
Sodium chloride (NaCl), potassium chloride (KCl), and their  $^{37}\text{Cl}$  and  $^{41}\text{K}$  isotopologues



Ginsburg et al. 2019.

The presence of a **disk-outflow** system (Hirota et al. 2017) indicates that “Orion source I” is accreting, confirming its nature as a young, forming star.

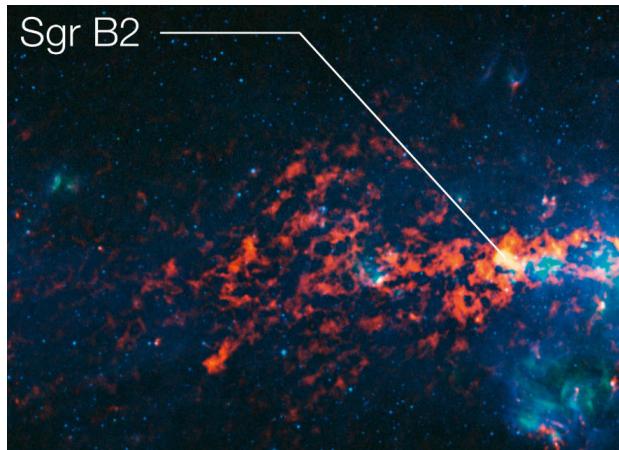
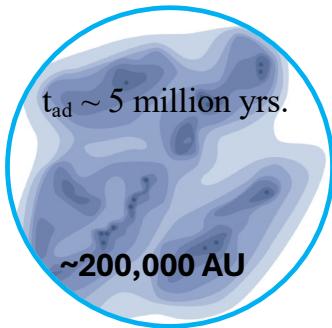
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# Molecular Line Data

## High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation

At the center of our galaxy,  
high mass clouds are  
chemically rich!



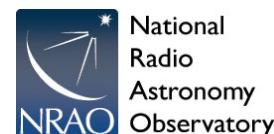
“Famous” cloud Sgr B2 is  
the #1 source of new  
molecule detections! Lots  
of complex chemistry!

McGuire 2022

# of molecule discoveries per source

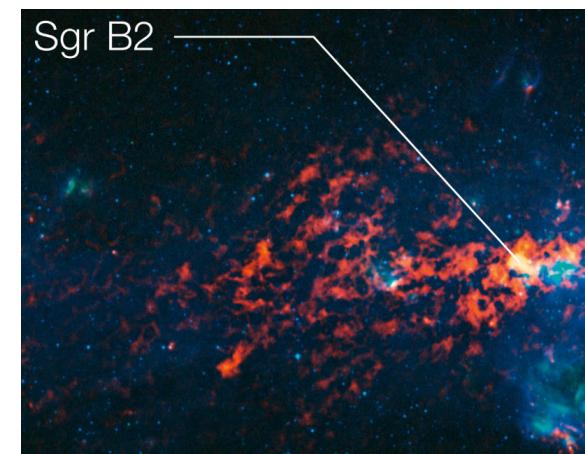
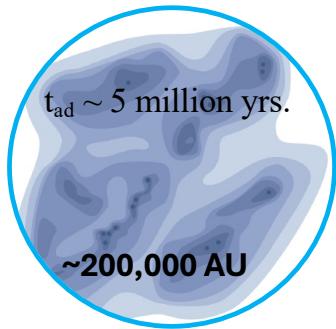
Source	#	Source	#
Sgr B2	69	L1527	2
TMC-1	57	L1544	2
IRC+10216	55	NGC 2024	2
LOS Cloud	42	NGC 7023	2
Orion	24	NGC 7027	2
L483	9	TC 1	2
W51	8	W49	2
VY Ca Maj	6	CRL 2688	1
B1-b	4	Crab Nebula	1
DR 21	4	DR 21(OH)	1
IRAS 16293	4	Galactic Center	1
NGC 6334	4	IC 443G	1
Sgr A	4	K3-50	1
CRL 618	3	L134	1
G+0.693-0.027	3	L183	1
NGC 2264	3	Lupus-1A	1
W3(OH)	3	M17SW	1
rho Oph A	3	NGC 7538	1
Horsehead PDR	2	Orion Bar	1

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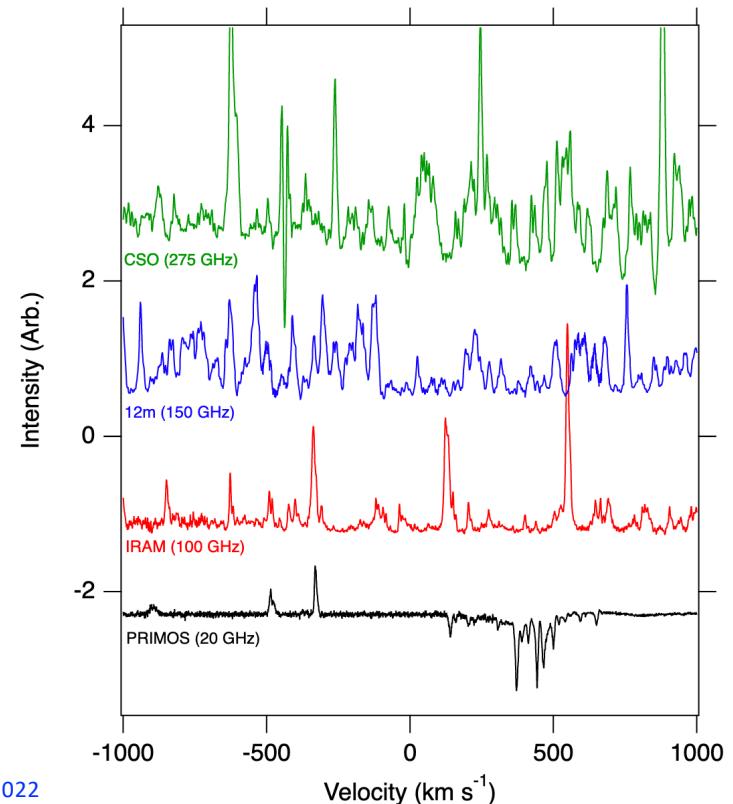
# Molecular Line Data

At the center of our galaxy,  
high mass clouds are  
chemically rich!



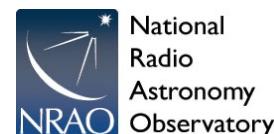
“Famous” cloud Sgr B2 is  
the #1 source of new  
molecule detections! Lots  
of complex chemistry!

High-mass ( $M > 8-10 M_\odot$ ) Star Formation



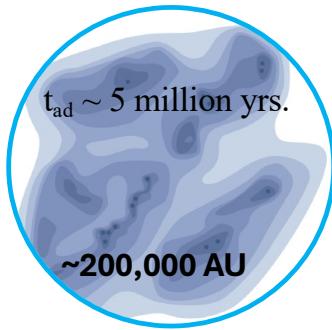
McGuire 2022

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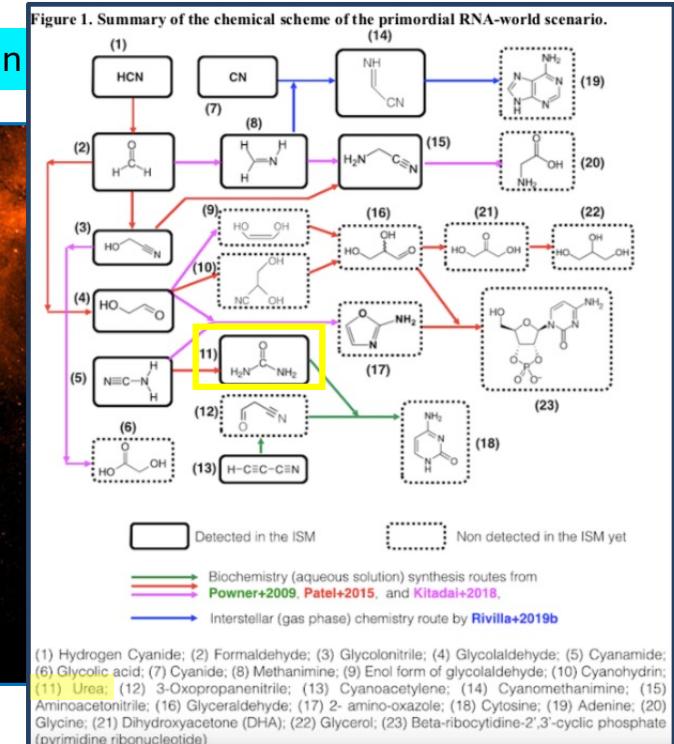
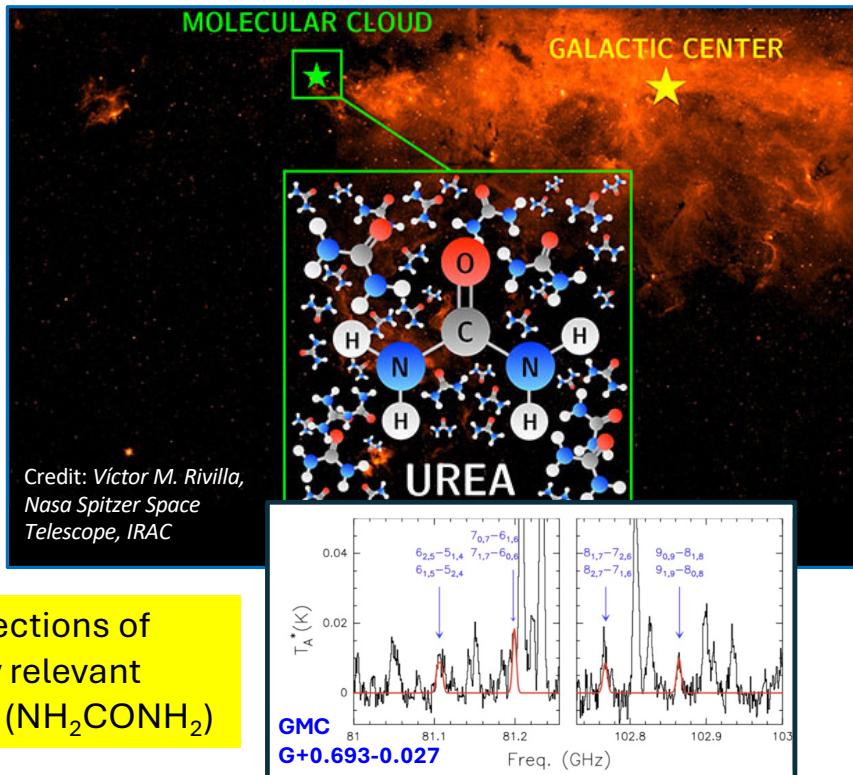


# Molecular Line Data

At the center of our galaxy, high mass clouds are chemically rich!

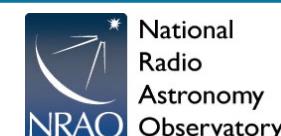


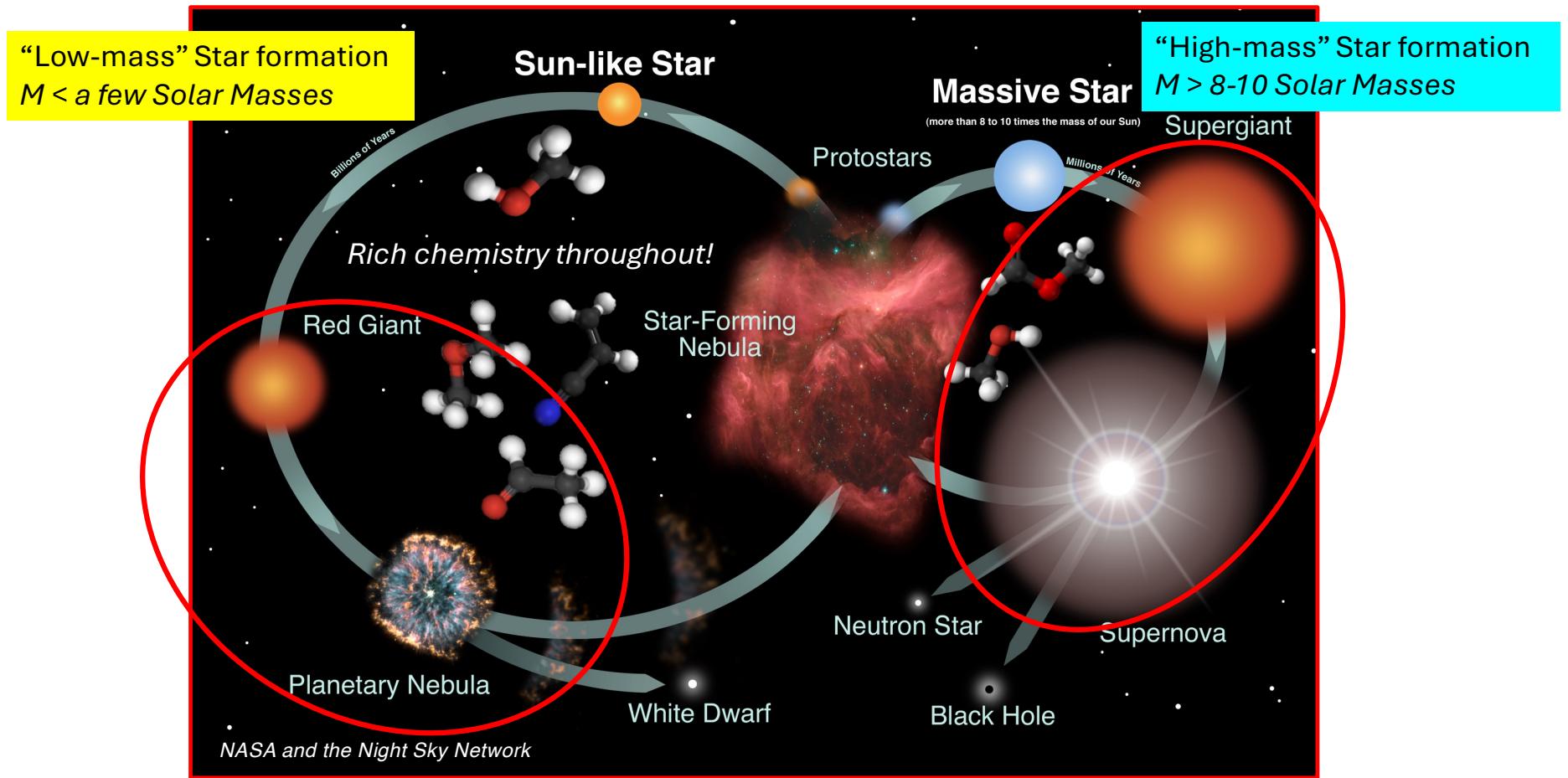
## High-mass ( $M > 8-10 M_{\odot}$ ) Star Formation



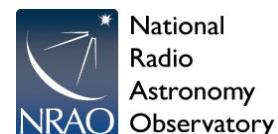
Jiménez-Serra et al. 2020

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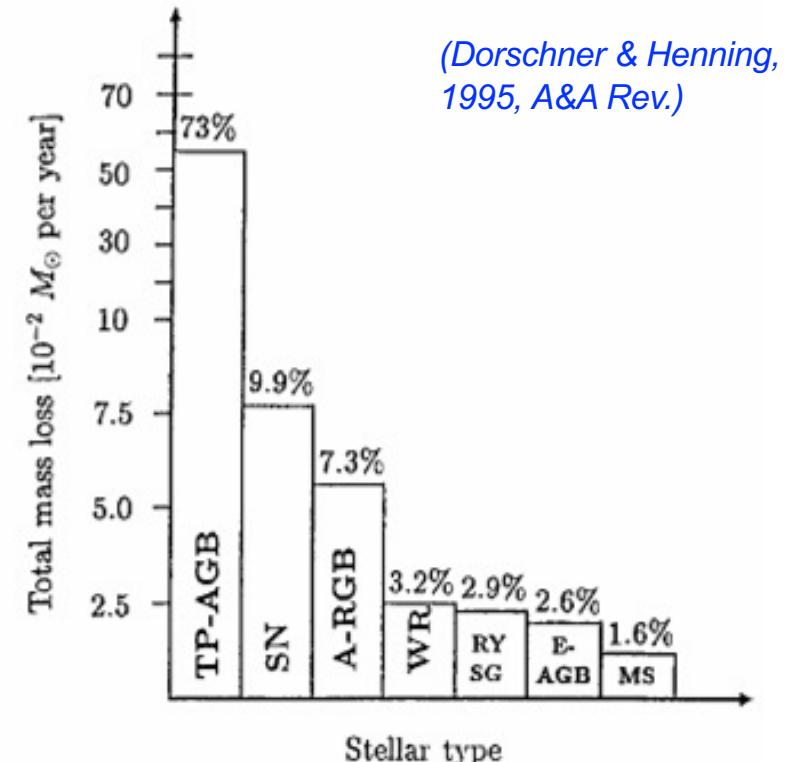


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## EVOLVED STARS

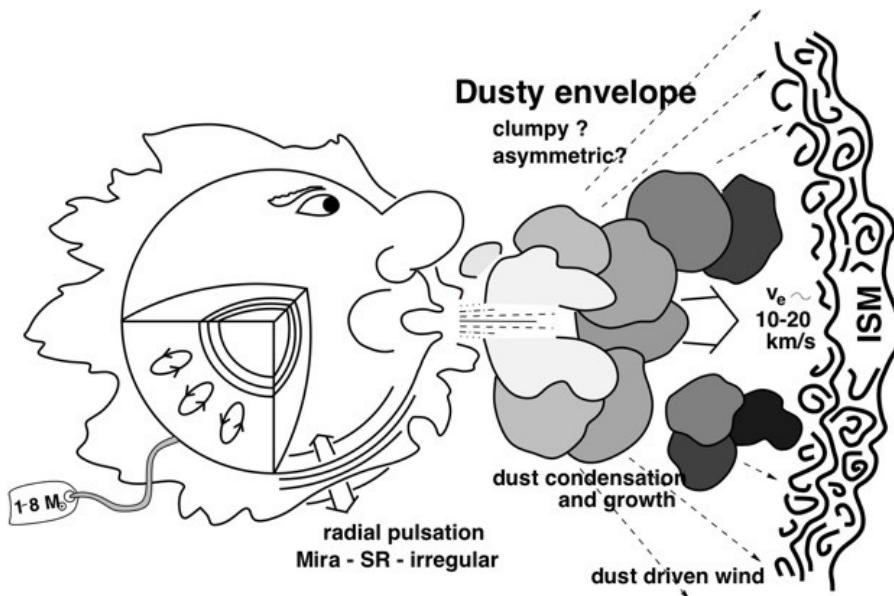
- **IMPORTANT** in astrochemistry because material is cycled back to the ISM!
- Mass loss from evolved stars  
    ⇒ ***Supplies 85% of material in ISM***
- Material cycled in  
***circumstellar shells of low-mass giants***
- Remainder from **Supernoave and Wolf-Rayet Stars**
- Material ends up in diffuse clouds
- Collapse to form **dense clouds**
- Important in evaluating
  - ⇒ Composition of **ISM**
  - ⇒ **Galactic Chemical Evolution**



Credit: L. Ziurys

## Molecular Line Data

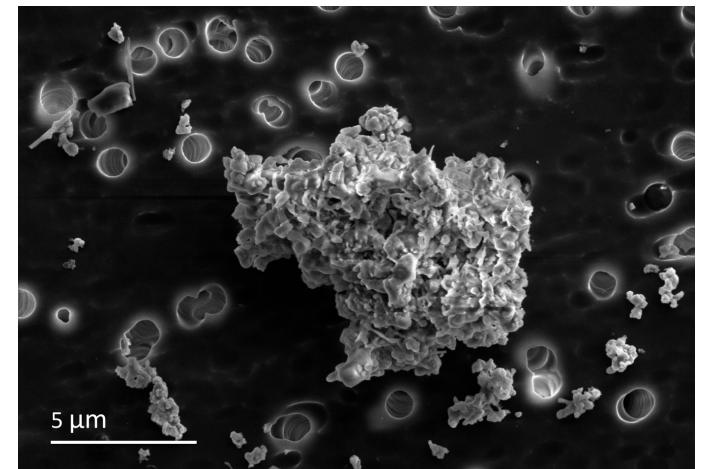
### Asymptotic Giant Branch (AGB) Stars



Olofsson 2011

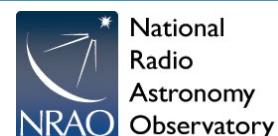
What does this mean for molecule formation?  
We know that where there is dust, molecules are likely form!!

Dust Grains born from material ejected from stars!



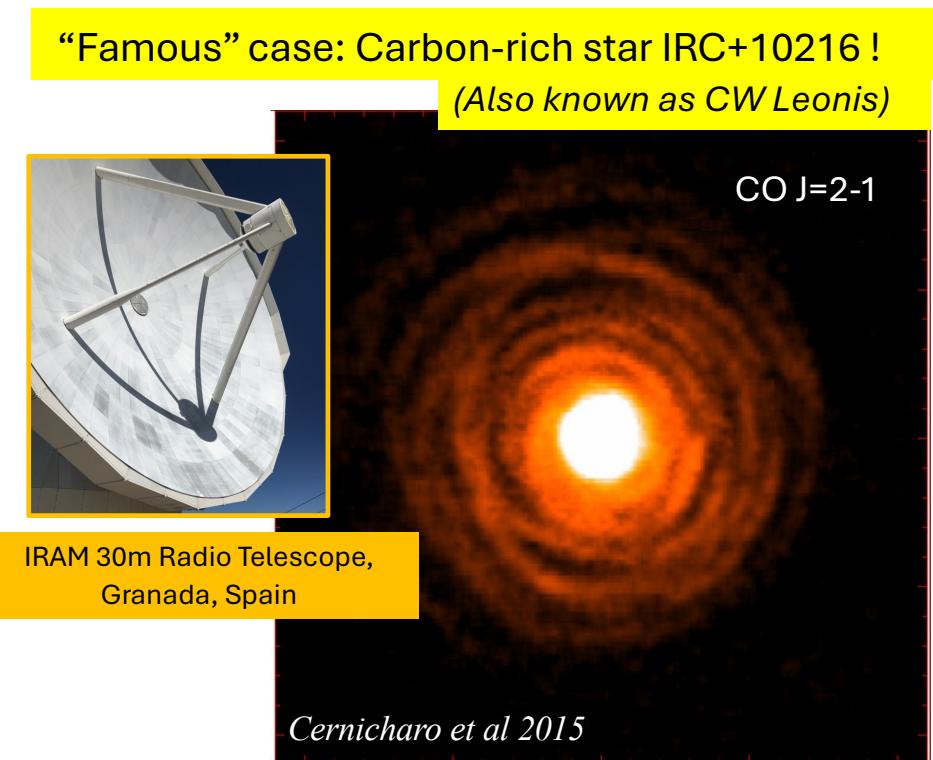
Credit: Hope Ishii, University of Hawai'i.

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## Molecular Line Data

### **Asymptotic Giant Branch (AGB) Stars**

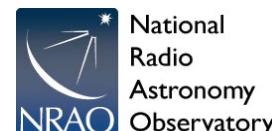


# of molecule discoveries per source

Source	#	Source	#
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B1-b	4	Crab Nebula	1
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NGC 6334	4	IC 443G	1
Sgr A	4	K3-50	1
CRL 618	3	L134	1
G+0.693-0.027	3	L183	1
NGC 2264	3	Lupus-1A	1
W3(OH)	3	M17SW	1
rho Oph A	3	NGC 7538	1
Horsehead PDR	2	Orion Bar	1

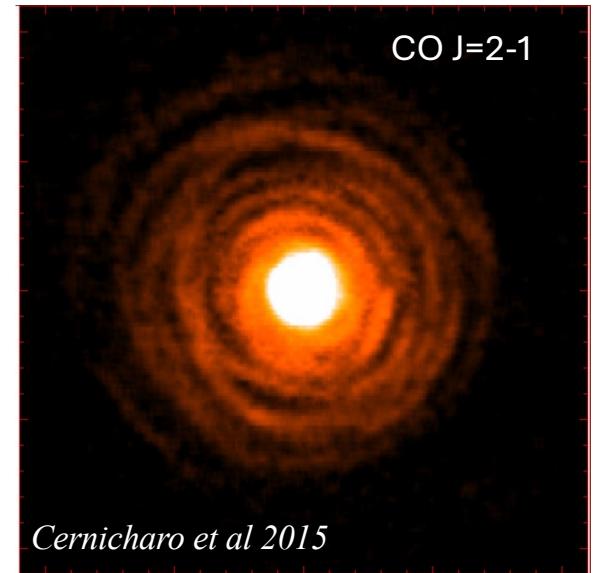
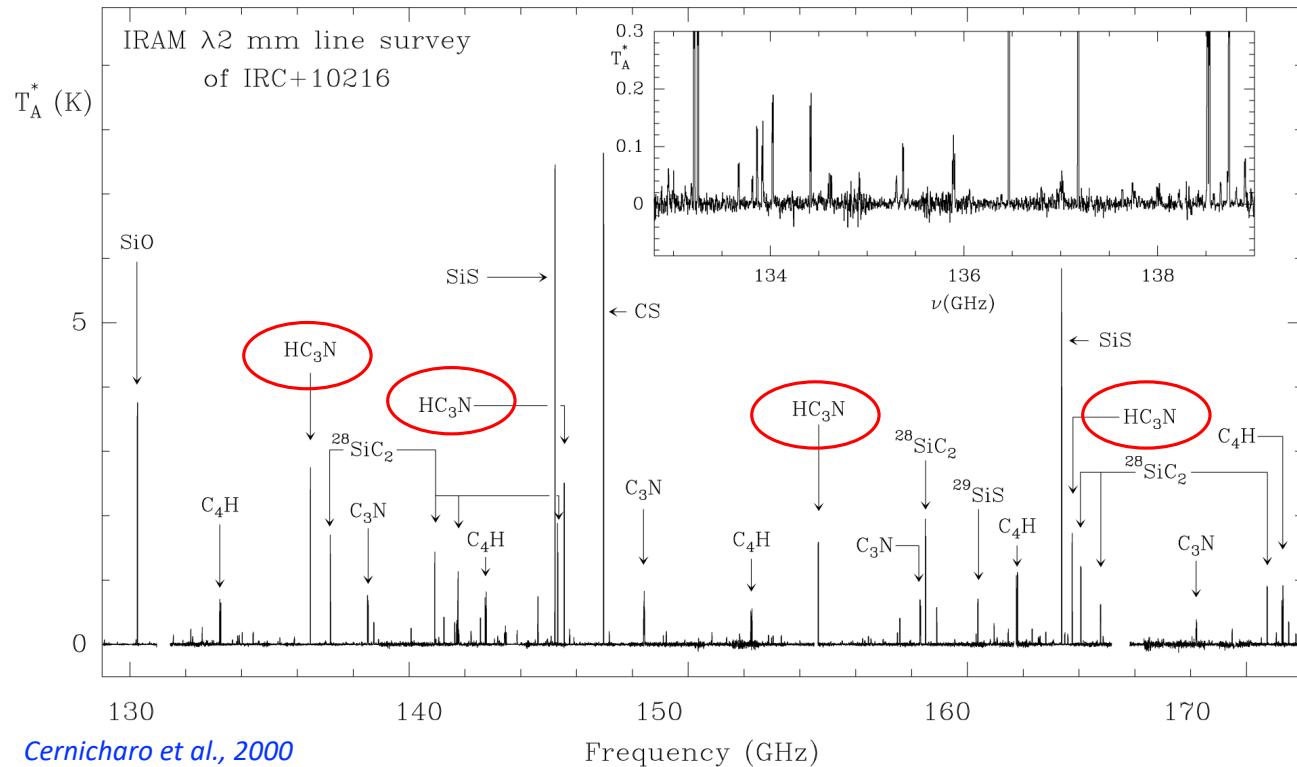
McGuire 2022

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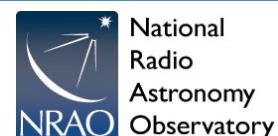
## Molecular Line Data

“Famous” case: Carbon-rich star IRC+10216 !



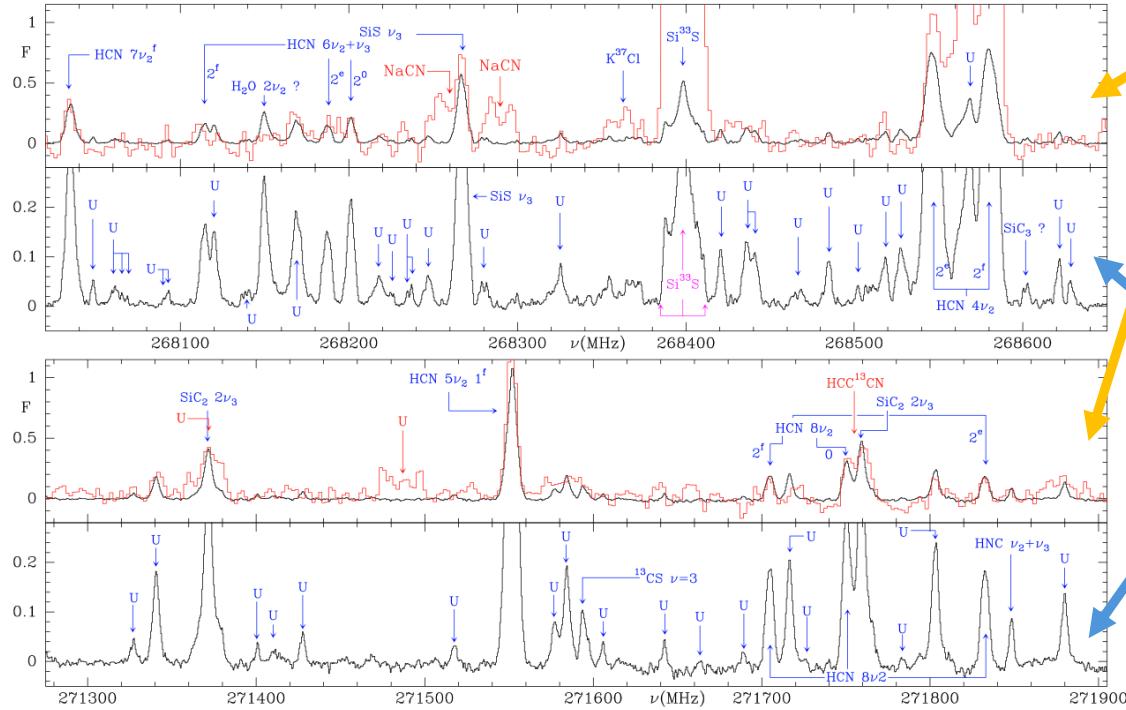
Rich in large carbon-chain  
and silicon-rich  
molecules!

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## Molecular Line Data

“Famous” case: Carbon-rich star IRC+10216 !



Cernicharo et al., 2013



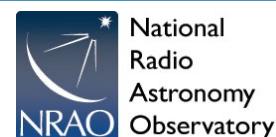
IRAM 30m Radio  
Telescope,  
Granada, Spain



ALMA interferometer

'Zooming in' with higher  
resolution and more sensitive  
telescope → Many 'U' lines,  
which are 'unidentified' !

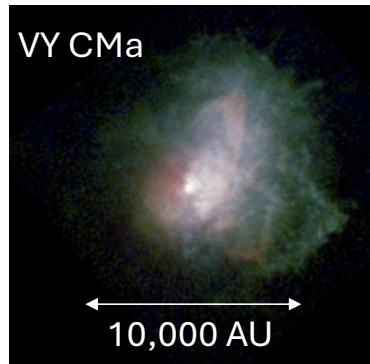
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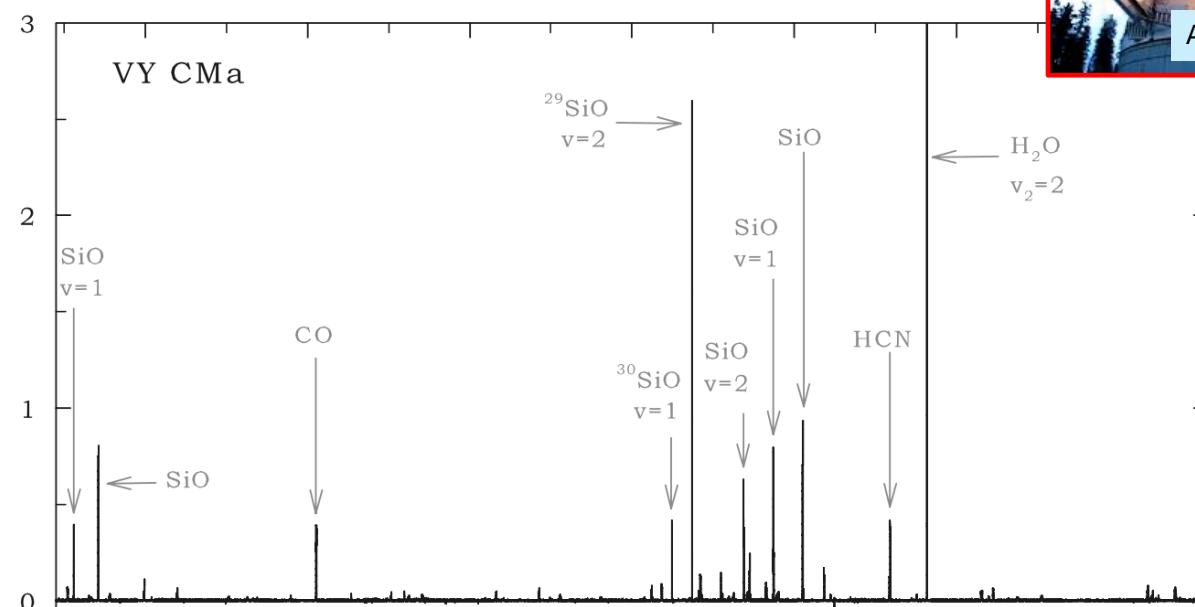
## Molecular Line Data

### *Supergiant Stars*

Oxygen-rich Supergiant star VY Canis Majoris

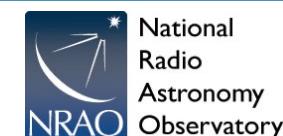


Tenenbaum et al., 2010

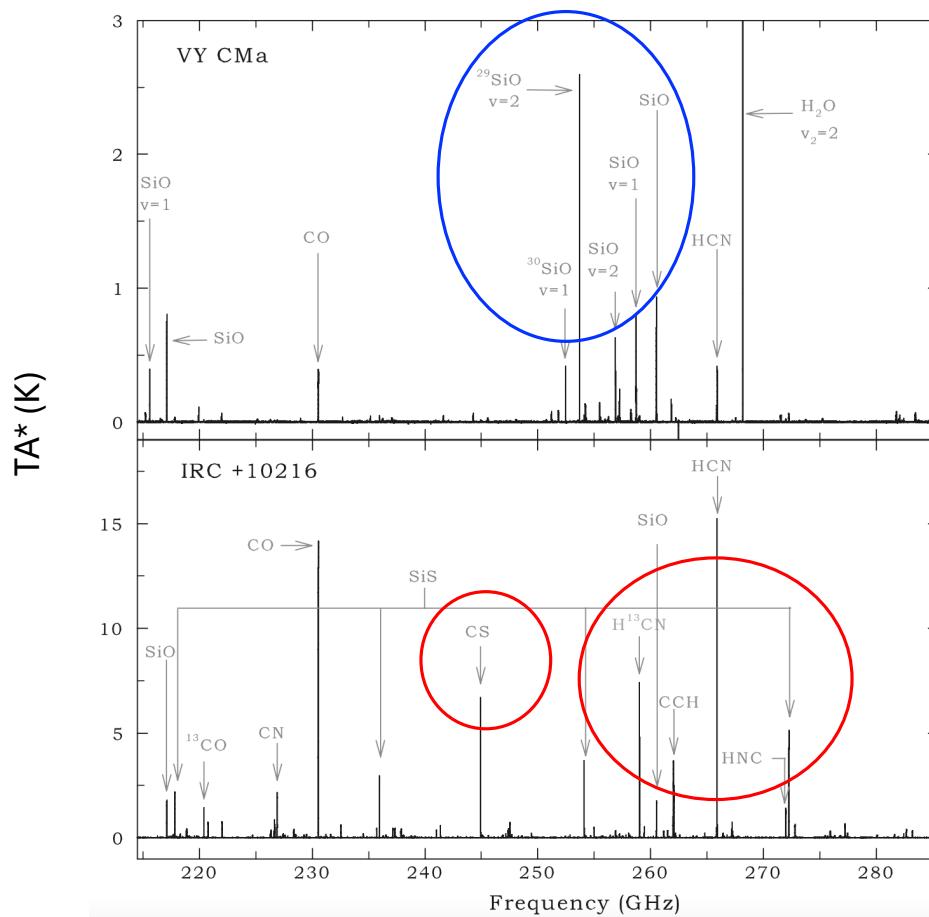
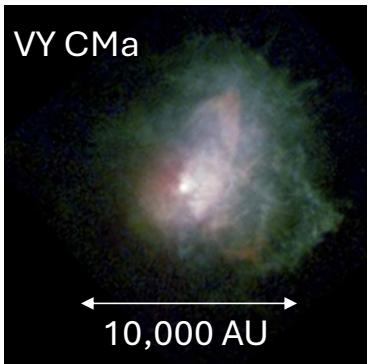


ARO 10m (SMT)

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# C-rich vs. O-rich

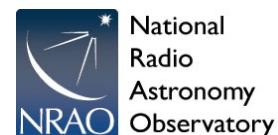


O-rich:  $\text{H}_2\text{O}$ ,  $\text{SiO}$ ,  $\text{CO}$

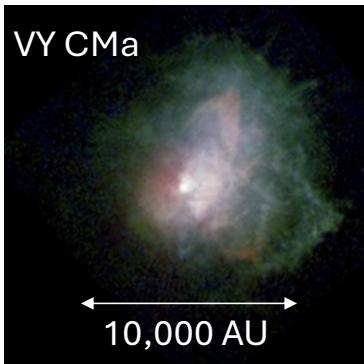
C-rich:  $\text{CO}$ ,  $\text{HCN}$ ,  
 $\text{H}_2\text{C}_2$ ,  $\text{SiS}$ ,  $\text{CS}$ ,  $\text{CH}_4$

Tenenbaum et al., 2010

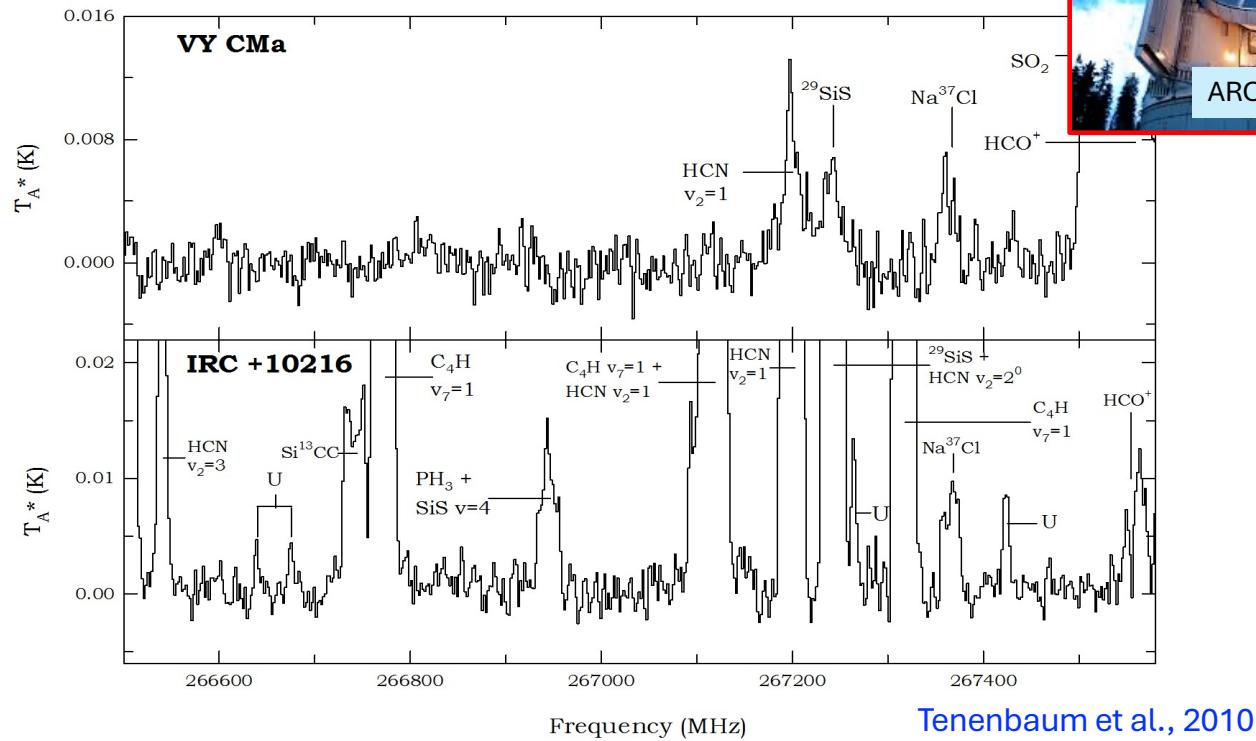
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# C-rich vs. O-rich

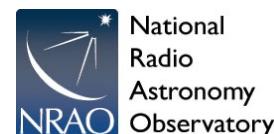


- VY CMa Spectrum dominated by **SO<sub>2</sub>, SiO, SiS**
- IRC+10216 Spectrum dominated by **C<sub>4</sub>H, HCN**

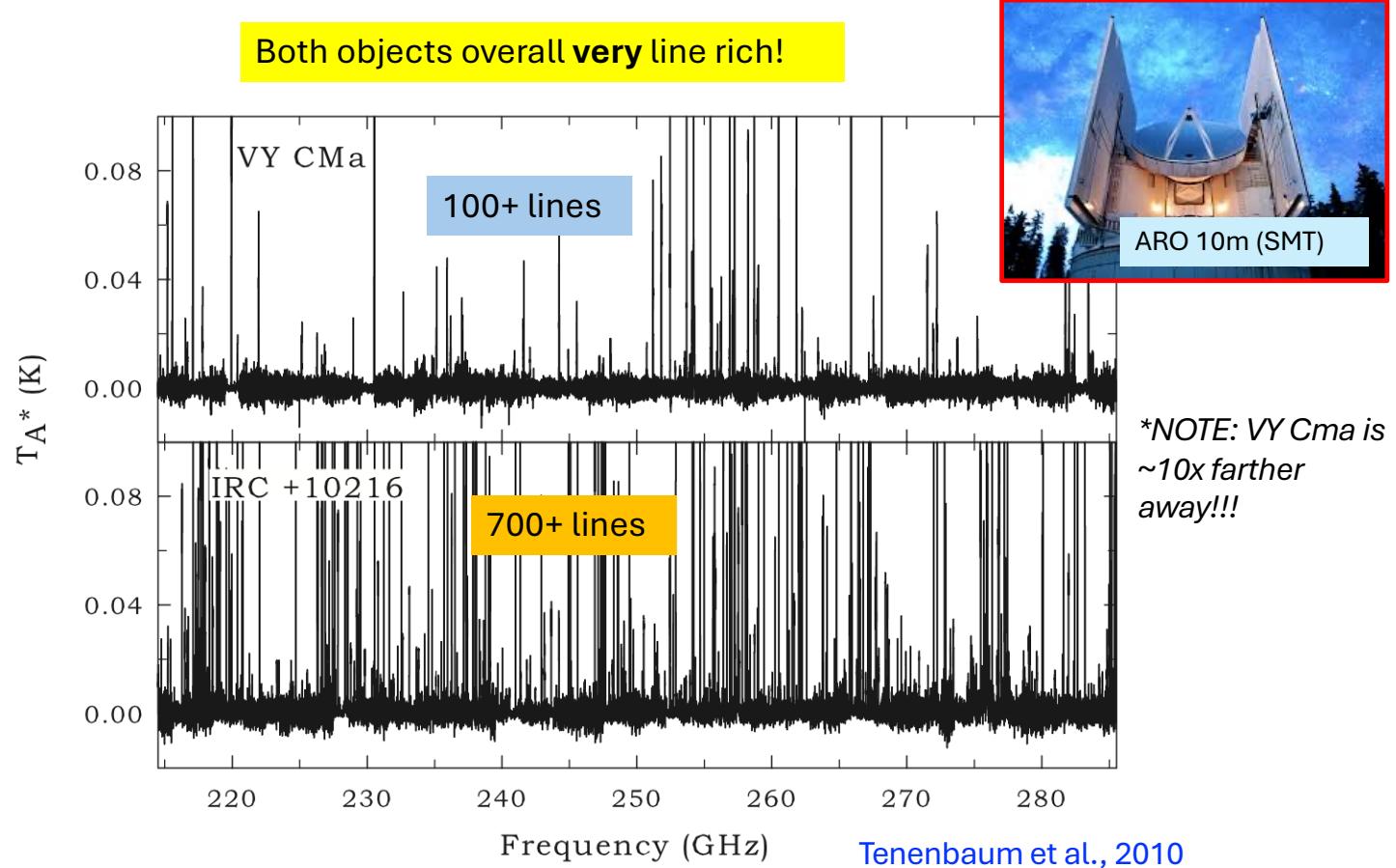
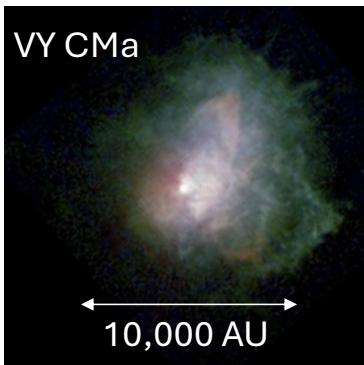


Tenenbaum et al., 2010

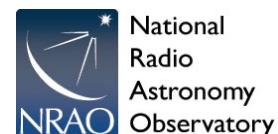
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# C-rich vs. O-rich

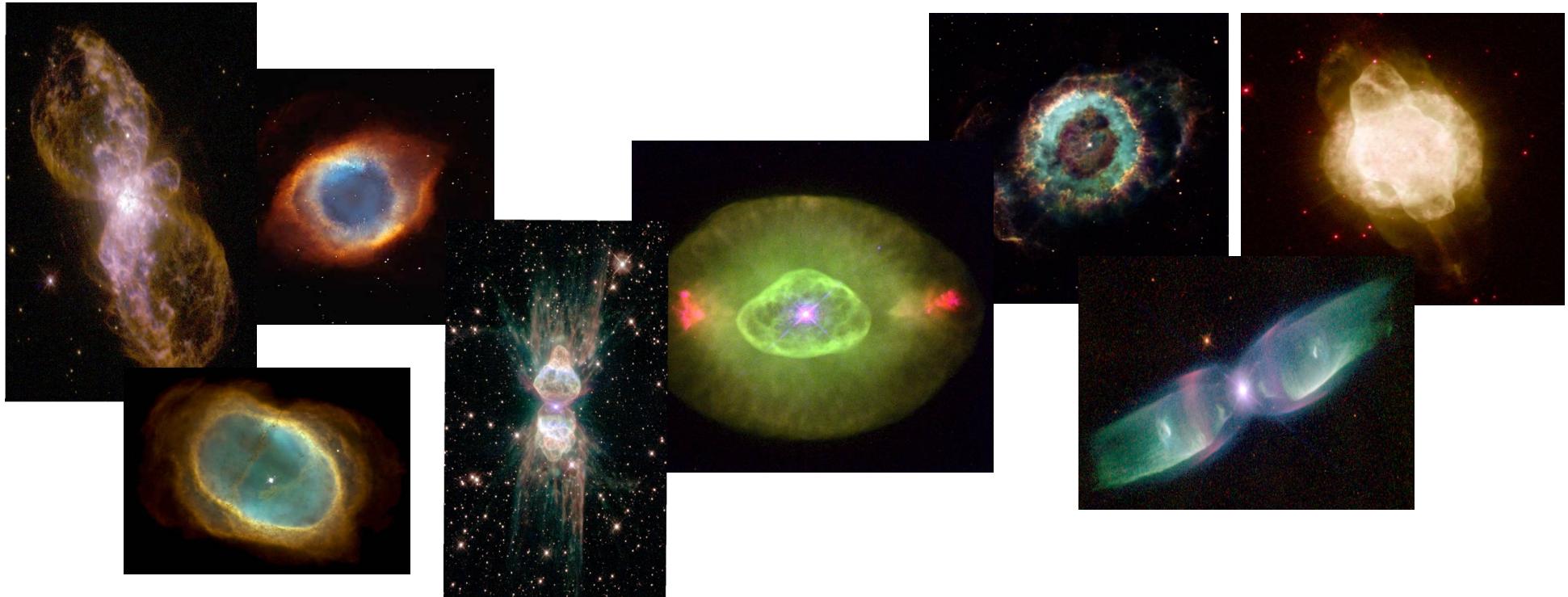


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## Molecular Line Data

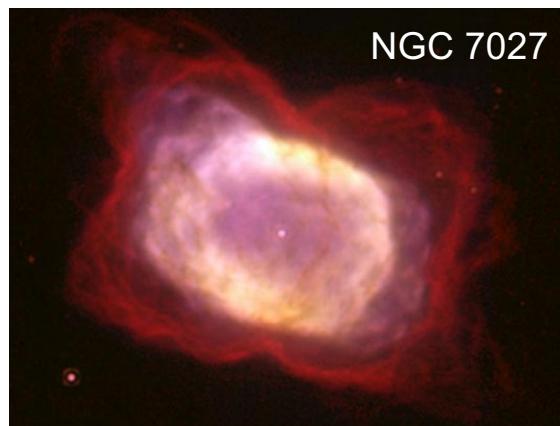
### *Planetary Nebula*



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## Molecular Line Data



Young PN: ~ **700 years old**  $T_{\text{star}} \sim 200,000 \text{ K}$

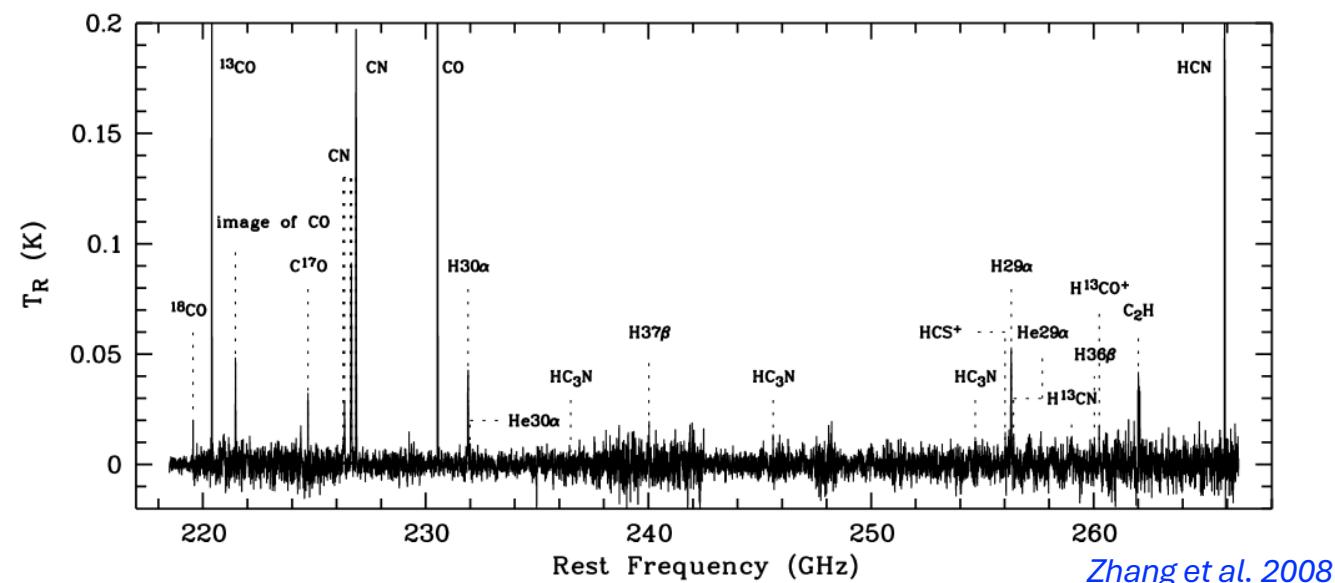
## *Planetary Nebula*

### Molecular Content:

CO, CN, HCN, HCO<sup>+</sup>, N<sub>2</sub>H<sup>+</sup>, CCH, C<sub>3</sub>H<sub>2</sub>, HC<sub>3</sub>N, OH, CH, CH<sup>+</sup>

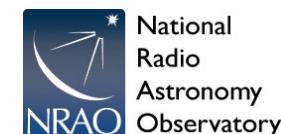


ARO 10m (SMT)



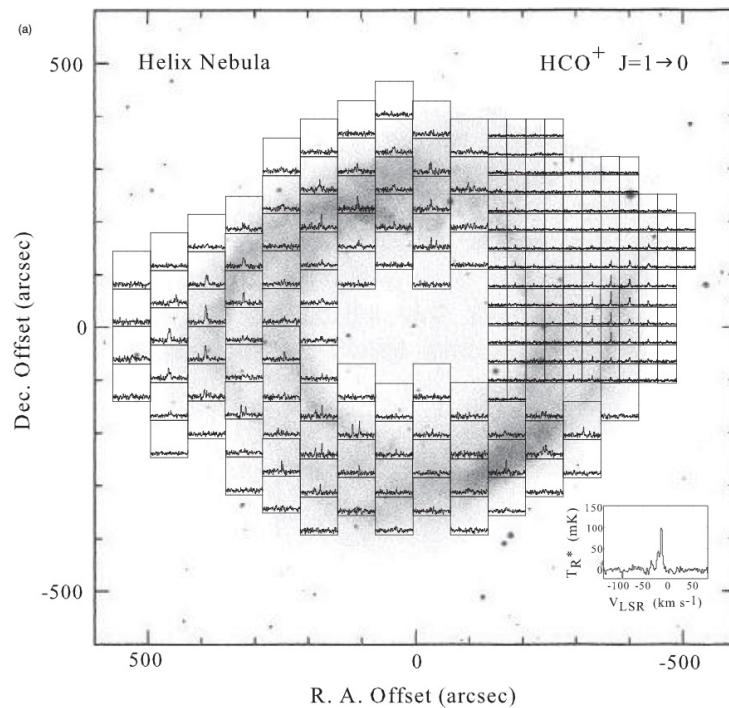
Zhang et al. 2008

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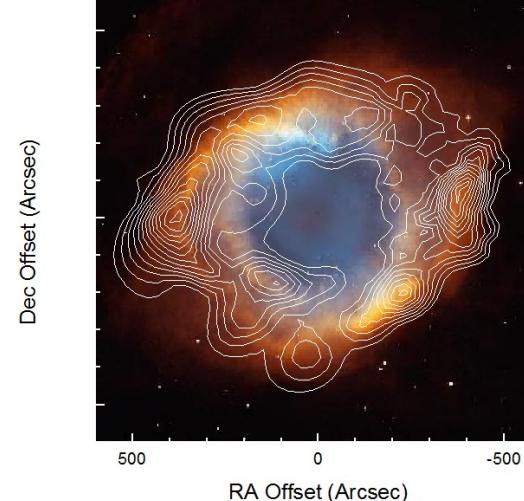


## Molecular Line Data

### Oldest Known Planetary Nebula: **The Helix**

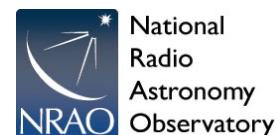


### *Planetary Nebula*



*Zeigler et al., 2013*

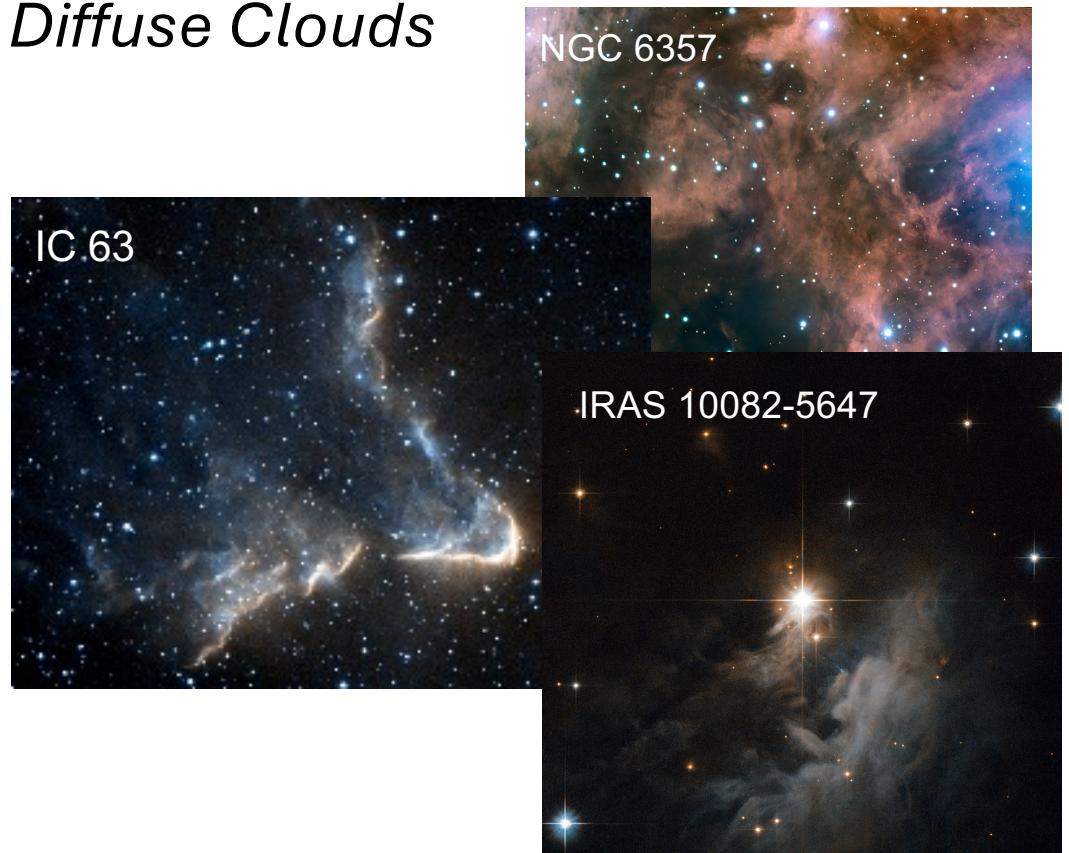
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Lack a *Definite Morphology*

- Semi-transparent in the visible ( $A_v \sim 1$ )
- Total hydrogen column density:  $N \sim 10^{21} \text{ cm}^{-2}$
- Readily penetrated by UV radiation

## Diffuse Clouds



Credit: L. Ziurys

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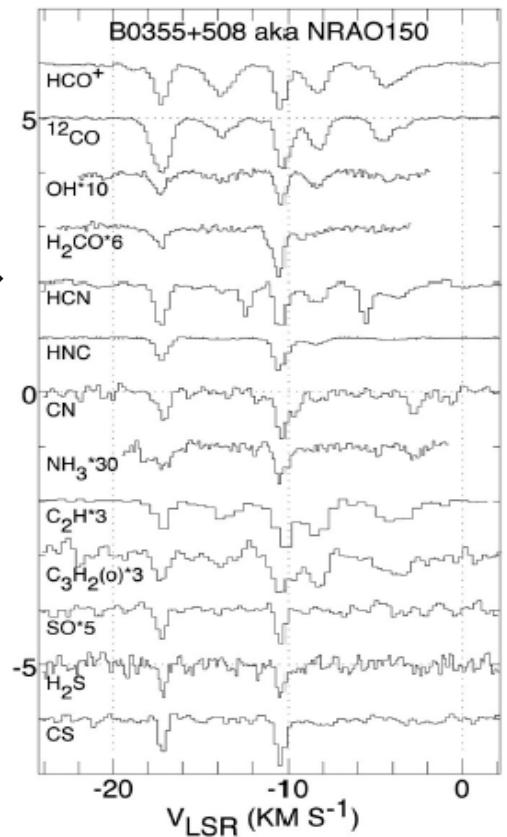
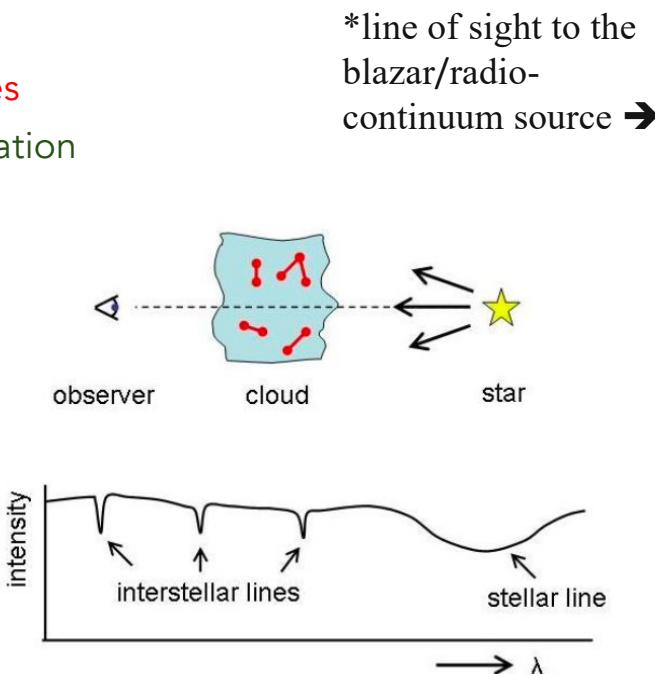


## Lack a *Definite Morphology*

- Semi-transparent in the visible ( $A_v \sim 1$ )
- Total hydrogen column density:  $N \sim 10^{21} \text{ cm}^{-2}$
- Readily penetrated by UV radiation
- Densities low: No radio/mm emission lines
- Not sufficient density for collisional excitation
- Molecules observed in ABSORPTION
- Common molecules observed
  - OH, H<sub>2</sub> (HD), CH, C<sub>2</sub>, CH<sup>+</sup>, NH,  
CO, H<sub>3</sub><sup>+</sup>

Credit: L. Ziurys

## Diffuse Clouds

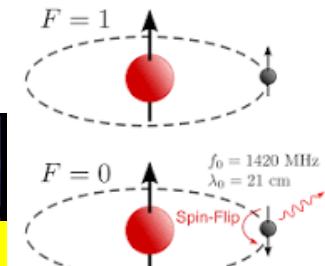
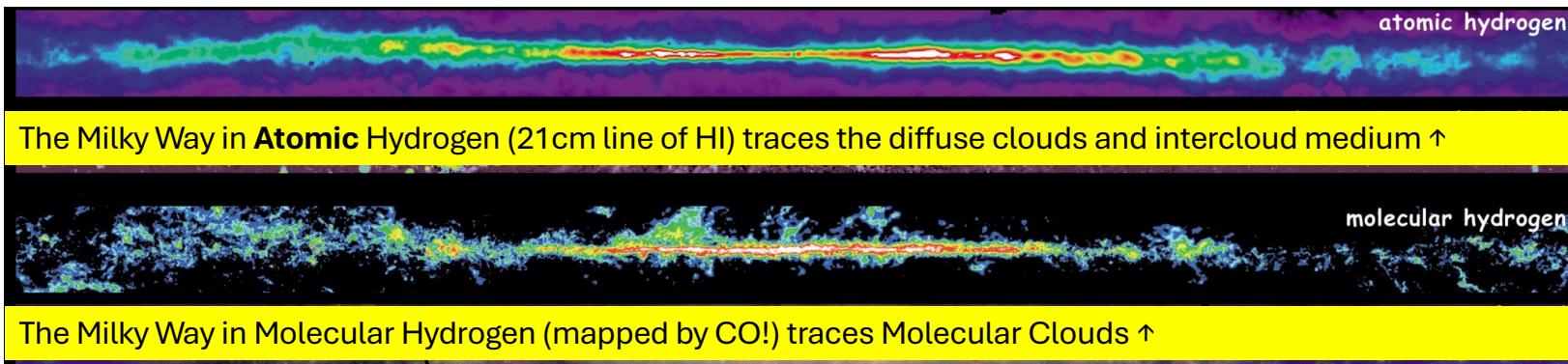


Lack a *Definite Morphology*

- Semi-transparent in the visible ( $A_v \sim 1$ )
- Total hydrogen column density:  $N \sim 10^{21} \text{ cm}^{-2}$
- Readily penetrated by UV radiation

## Diffuse Clouds

- Best traced by **21 cm HI line**
- $T_k \sim 100 \text{ K}$
- $n \sim 1 - 100 \text{ particles/cm}^3$  ( $H^0 + H_2$ )
- $x_e \sim 10^{-3}$  (*Fractional ionization*)



**Reminder!** Typical Conditions of Molecular Clouds:  $T \sim 10 - 50 \text{ K}$ ;  $n \sim 10^3 - 10^6 \text{ cm}^{-3}$

Credit: L. Ziurys

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