

VENUE:

**Department of
Physics and
Astronomy**

Galileo Galilei
Institute for
Theoretical Physics



ASTR 5340 - Introduction to Radio Astronomy
Contact: sscibell@nrao.edu



Fractionation of isotopes in space II
from the Solar System to galaxies
 November 4th to 7th 2024 - Florence, Italy



Views!

Foods!

Cats!

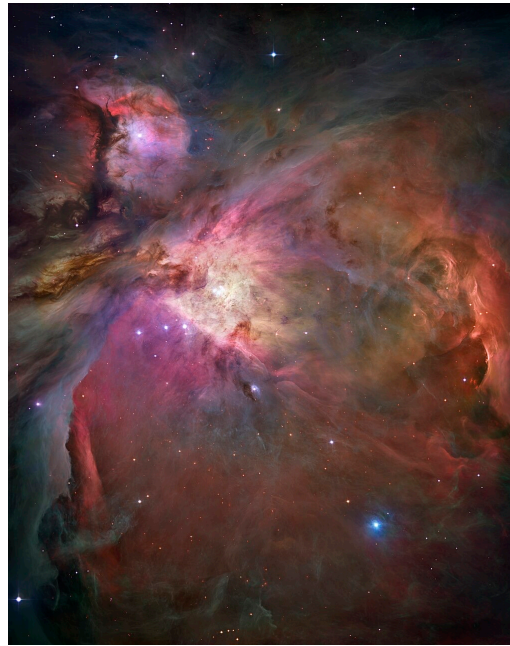


Emission Mechanisms

Spectral Lines (ERA Chap. 7)



Free-Free (ERA Chap. 4)



Synchrotron (ERA Chap. 5)



Pulsars (ERA Chap. 6)



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Emission Mechanisms

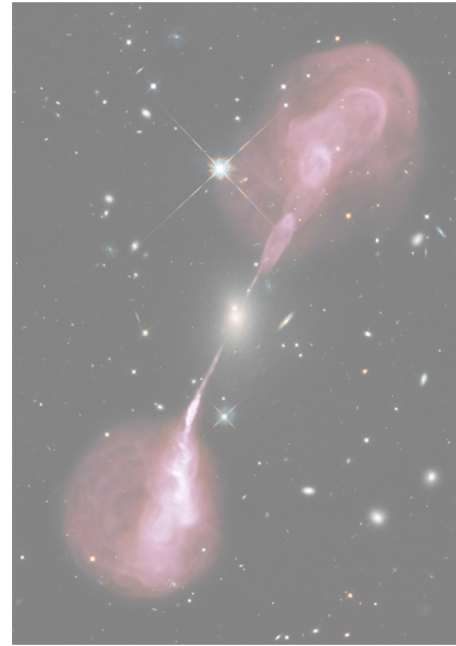
Spectral Lines (ERA Chap. 7)



Free-Free (ERA Chap. 4)



Synchrotron (ERA Chap. 5)



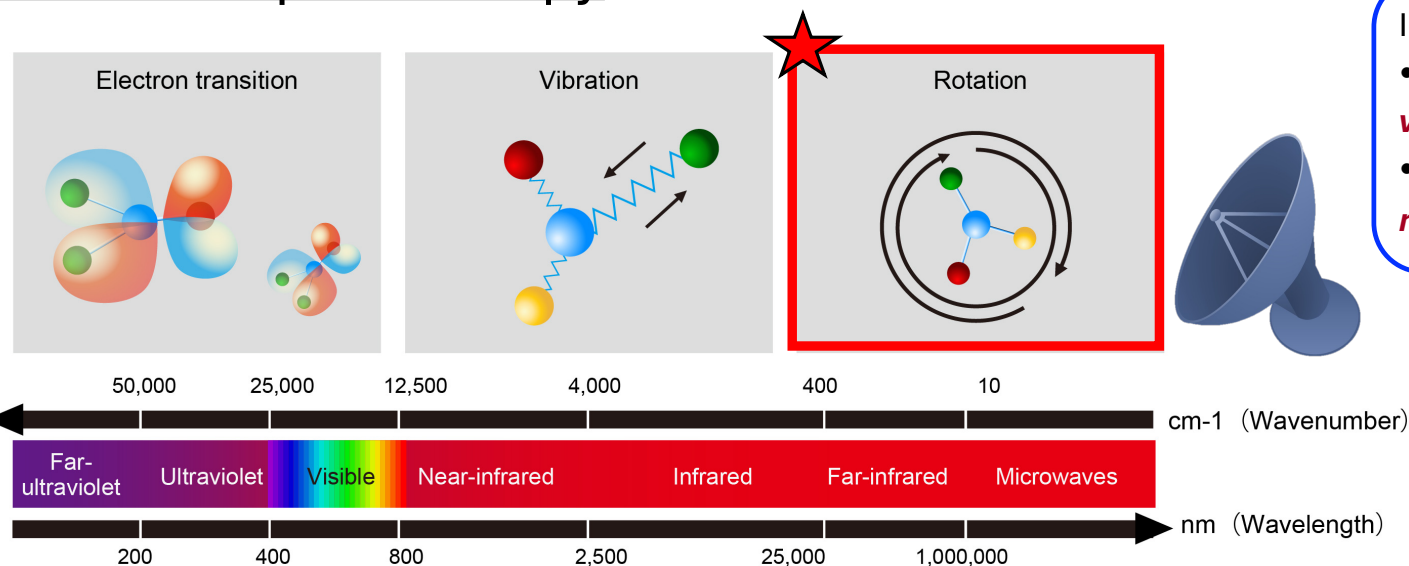
Pulsars (ERA Chap. 6)



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Submillimeter and Millimeter Radio Telescopes Identify Molecules via Rotational Spectroscopy!



Important to know all because...

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

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

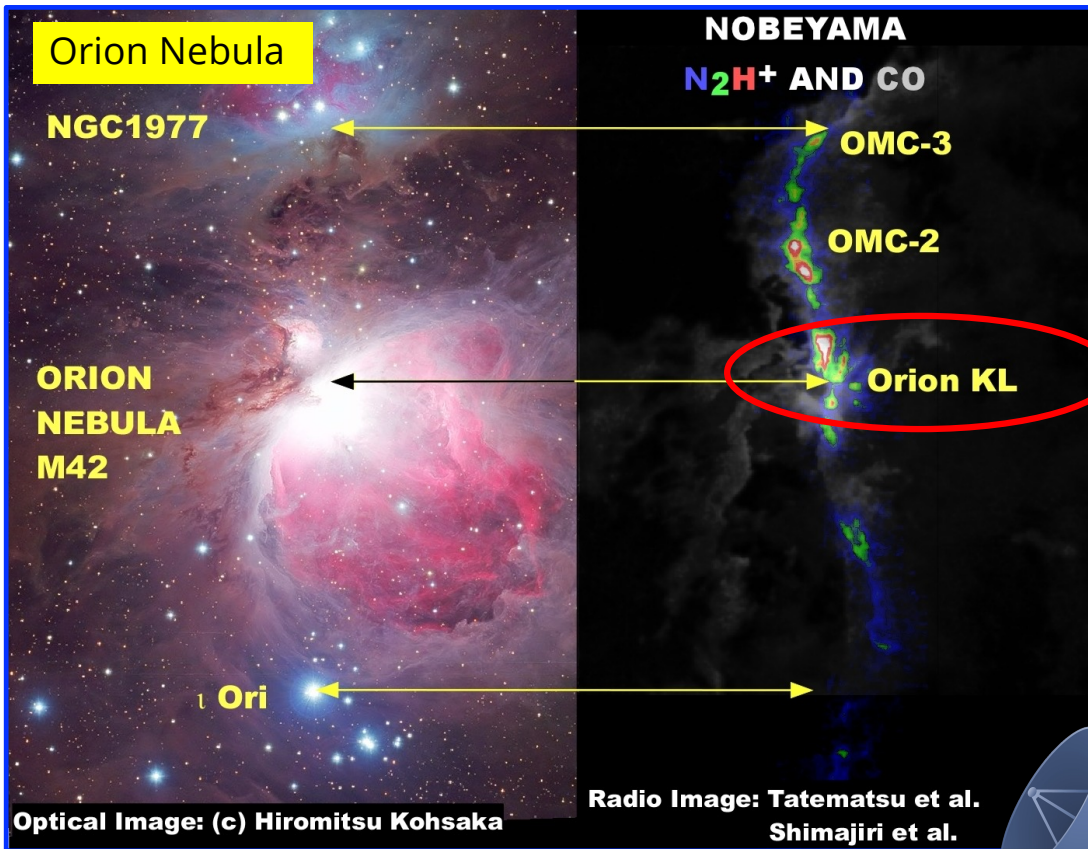
- end-on-end motion of nuclei
- energies in microwave/millimeter-wave regions

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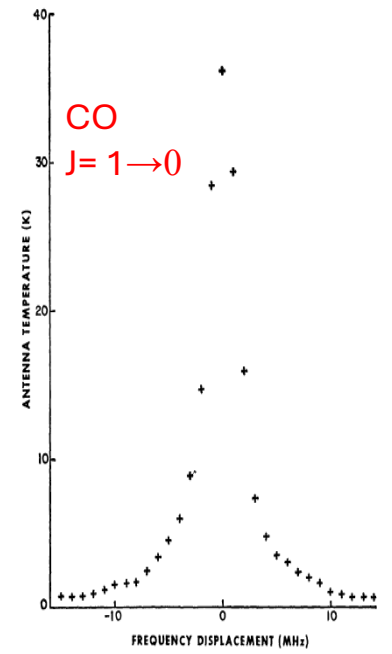
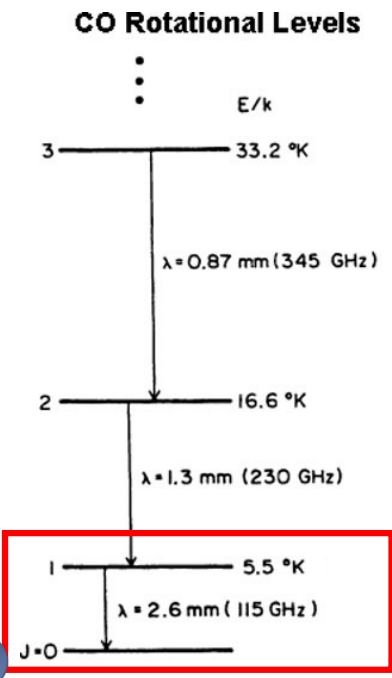
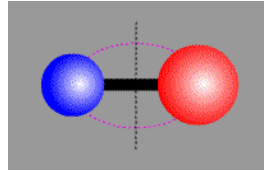
National Radio Astronomy Observatory



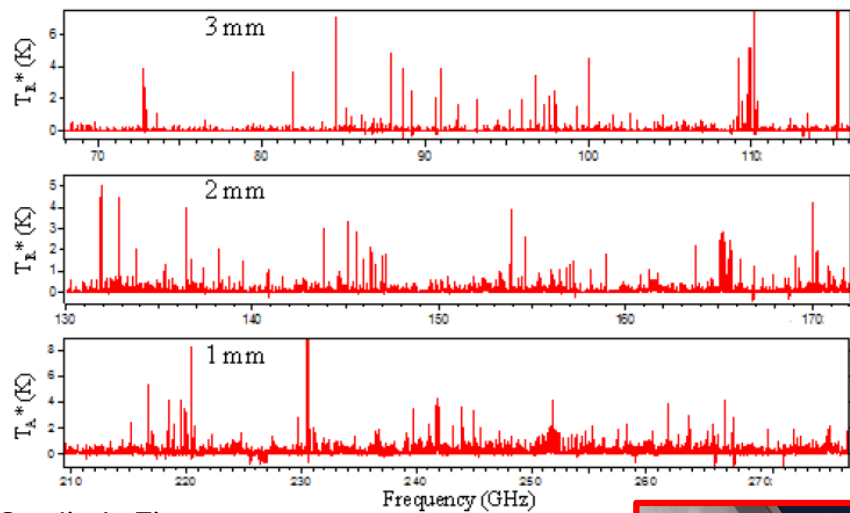


<https://www.nro.nao.ac.jp/~kt/html/kt-e.html>

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

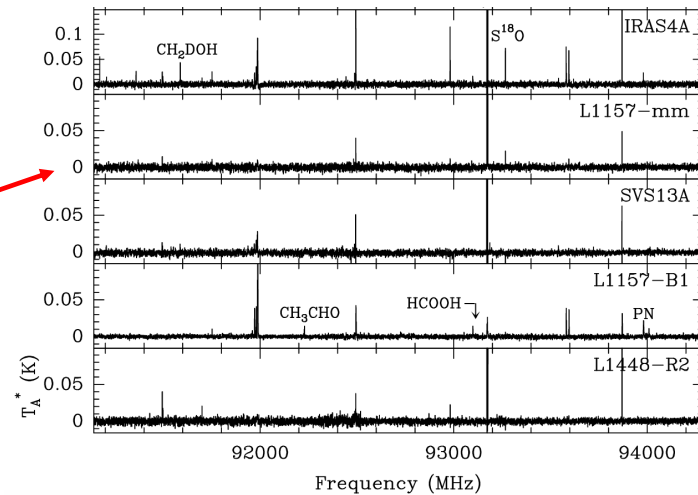
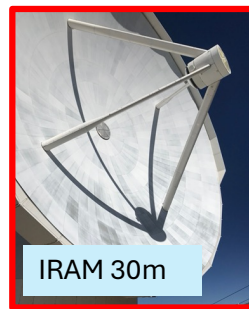


Rotational Lines of Molecules at Radio Wavelengths



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_{χ}):

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

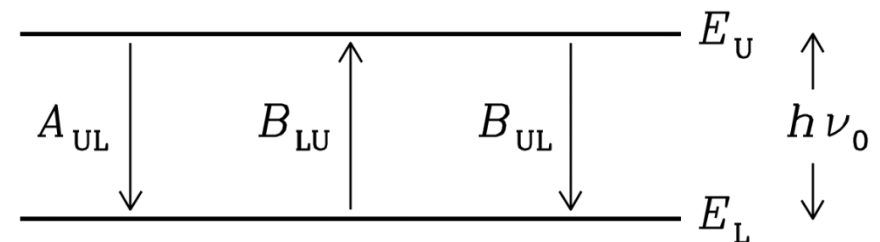
* When $T_{\text{ex}} \sim T_{\text{k}}$ then LTE a good approximation!

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

Optically thin lines (e.g., ^{13}CO or C^{18}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 **Splatalogue!**

<https://splatalogue.online>

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

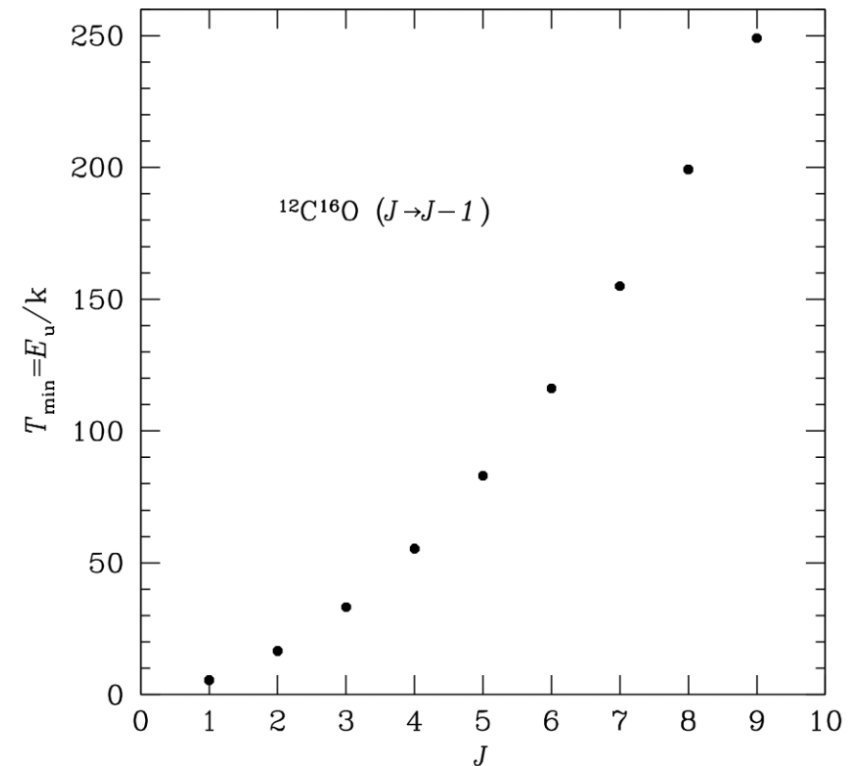
*Key Things to Remember!

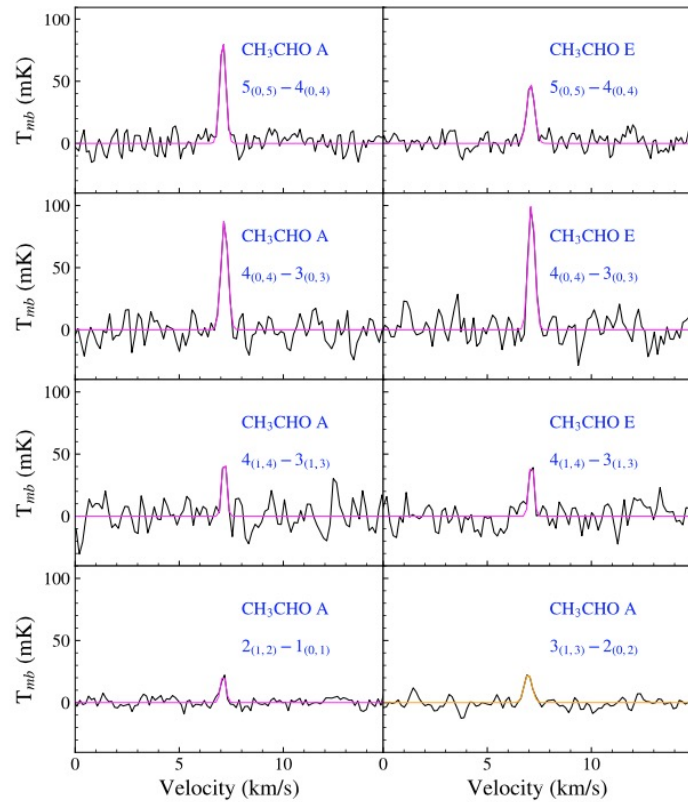
Related to A_{UL} , the **upper energies** give clues into what type of environments are molecular lines are likely to emit at and are directly connected to the minimum gas temperature needed for significant collisional excitation,

$$T_{\min} \sim \frac{E_{\text{rot}}}{k}$$
$$\sim \frac{J(J+1)h^2}{2 \cdot 4\pi^2 I k} = \frac{hJ}{4\pi^2 I} \frac{h(J+1)}{2k} = \frac{E_U}{k}$$

(7.116 & 7.118)

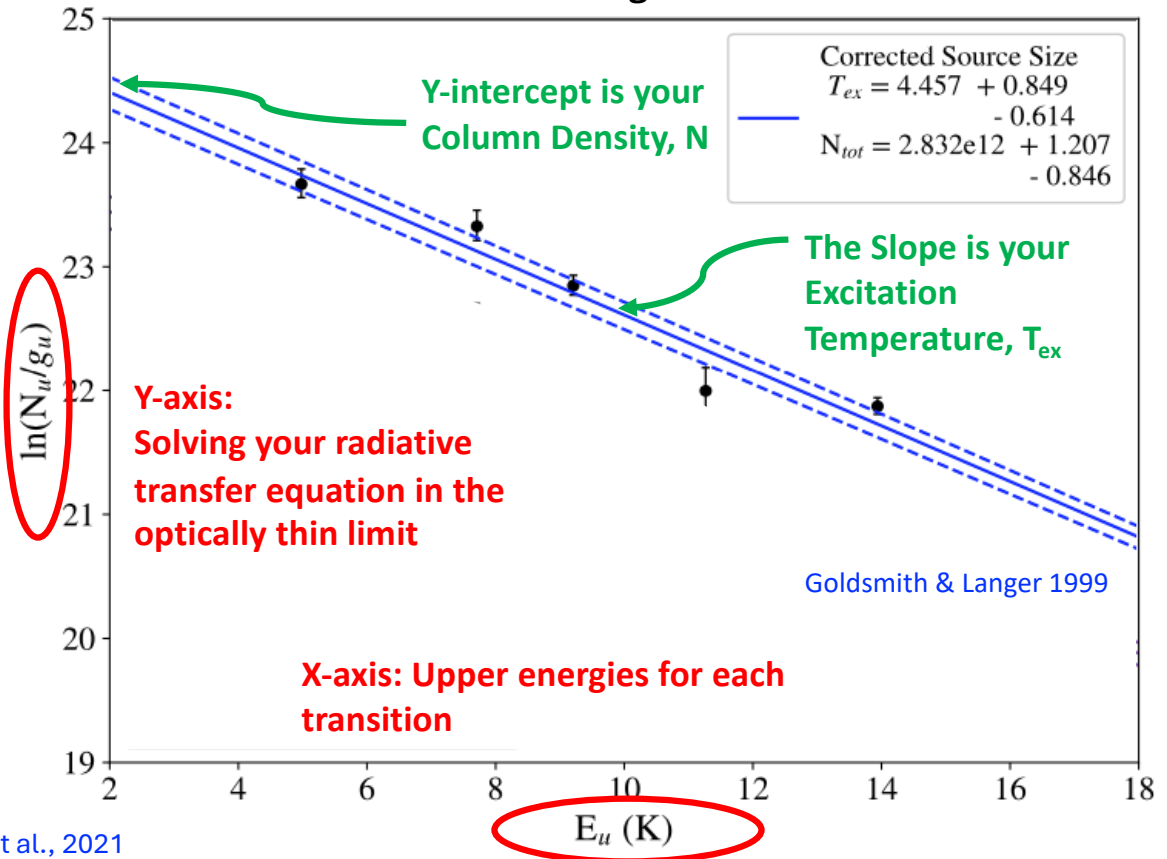
Fig. 7.15 (ERA)





Scibelli et al., 2021

Practical use → Rotation Diagrams

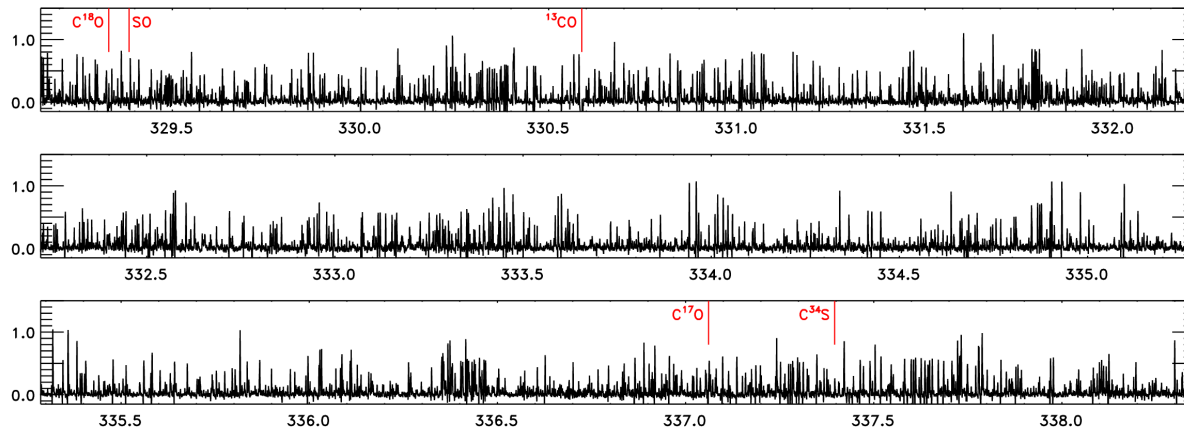


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Isotopologues (ERA 7.7)

“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.,

$C^{18}O$, ^{13}CO , $C^{17}O$, $C^{34}S$, $H^{13}CO^+$, $HC^{18}O^+$, $H^{13}CN$, $H^{15}CN$, ^{29}SiO , $^{13}CH_3OH$, DCN , DCO^+

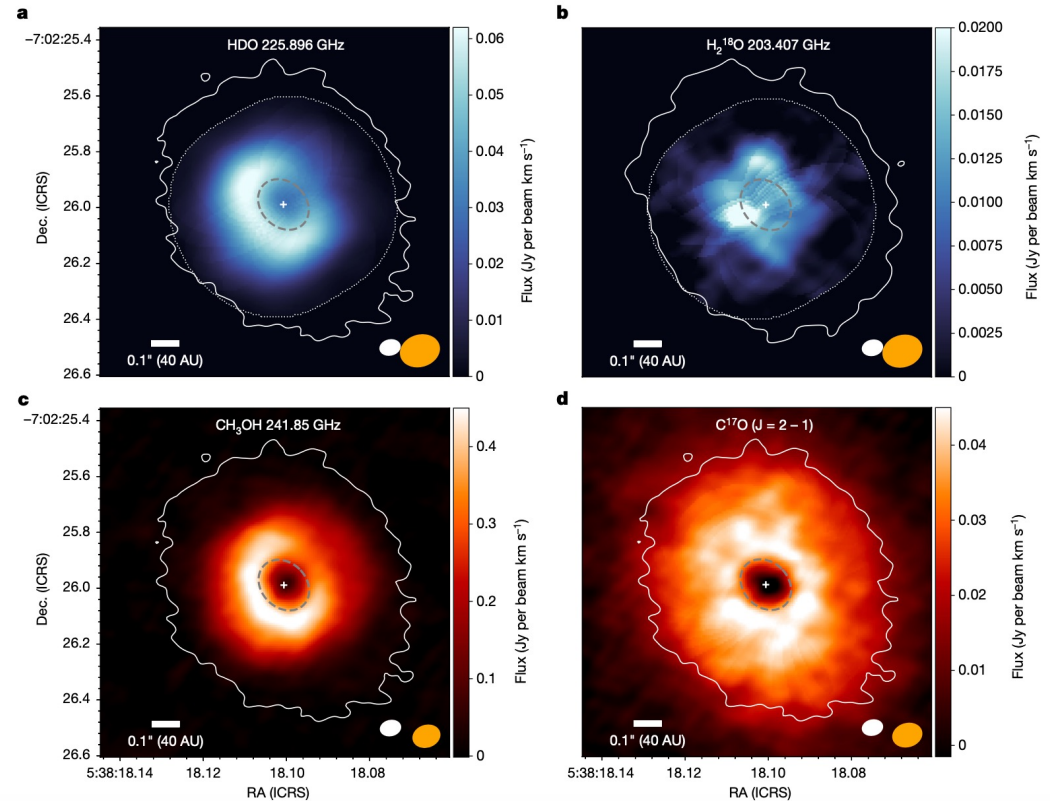
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Isotopologues (ERA 7.7)

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***



disk of V883 Ori

Tobin 2023, Nature

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Isotopologues (ERA 7.7)

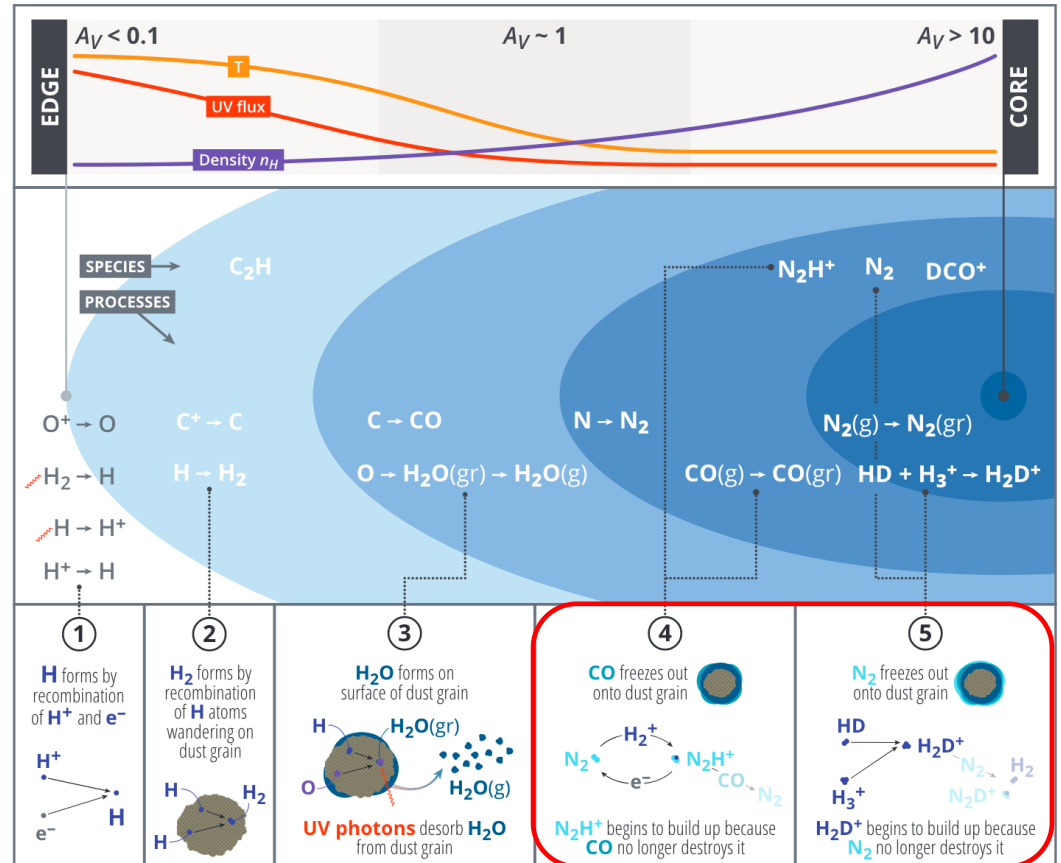
Benefits of observing Isotopes:

- ***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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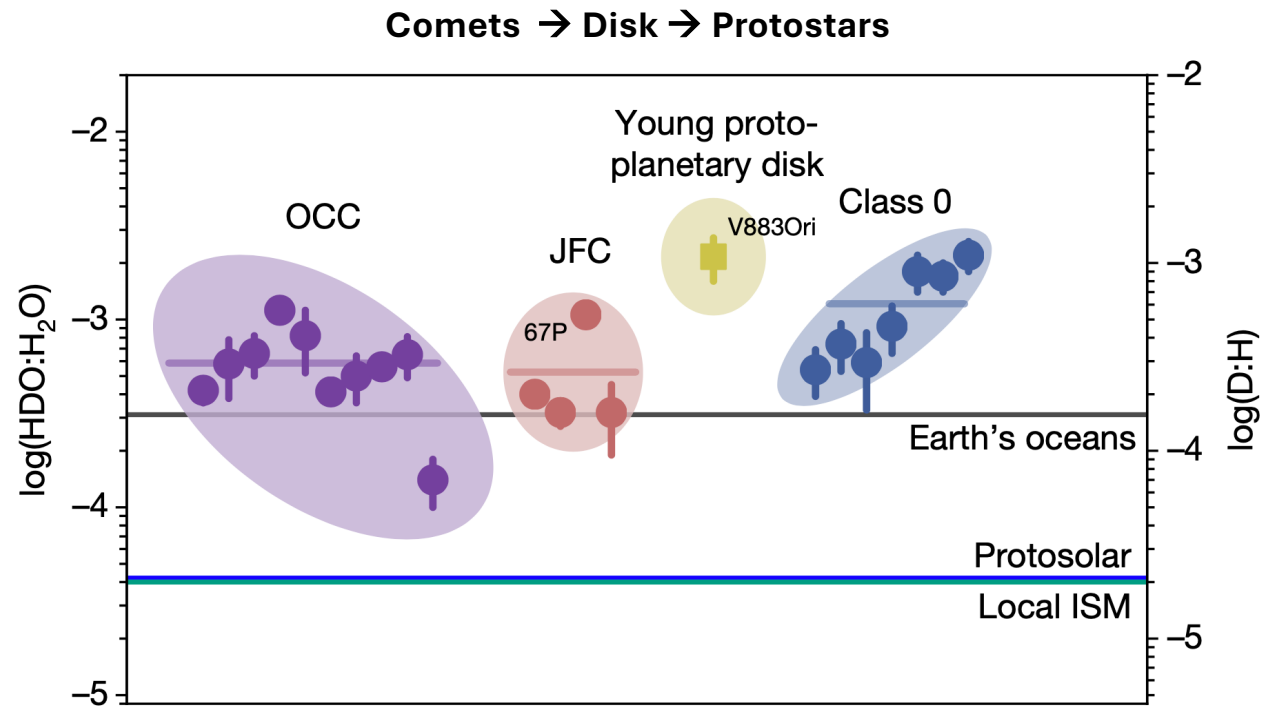
National Radio Astronomy Observatory



Isotopologues (ERA 7.7)

HDO:H₂O ratio does not strongly evolve from the protostar phase to the disk!

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

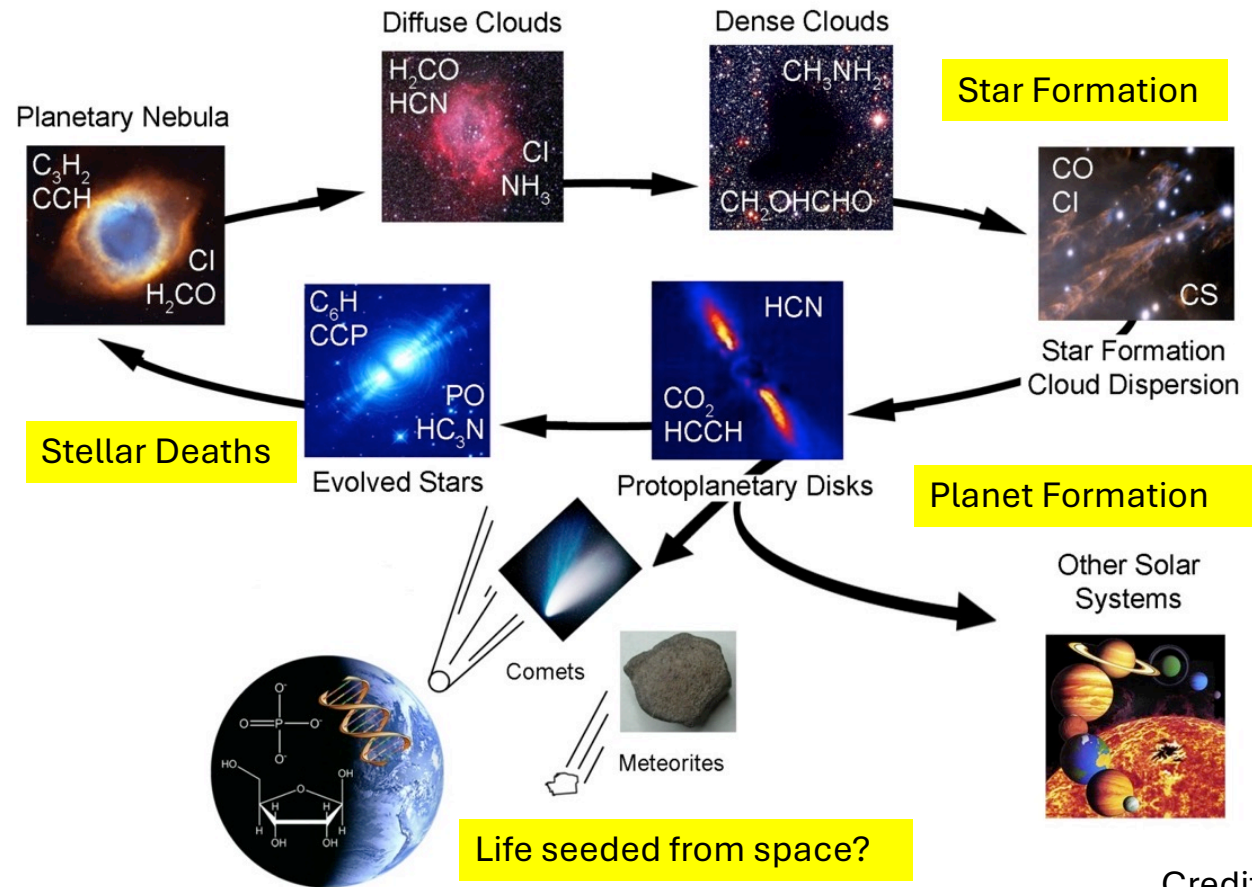


Tobin 2023, Nature

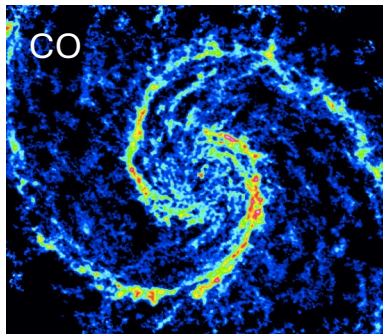
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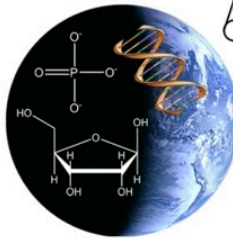
Molecular Life Cycle



Within Galaxies... →



M51 – Whirlpool Galaxy



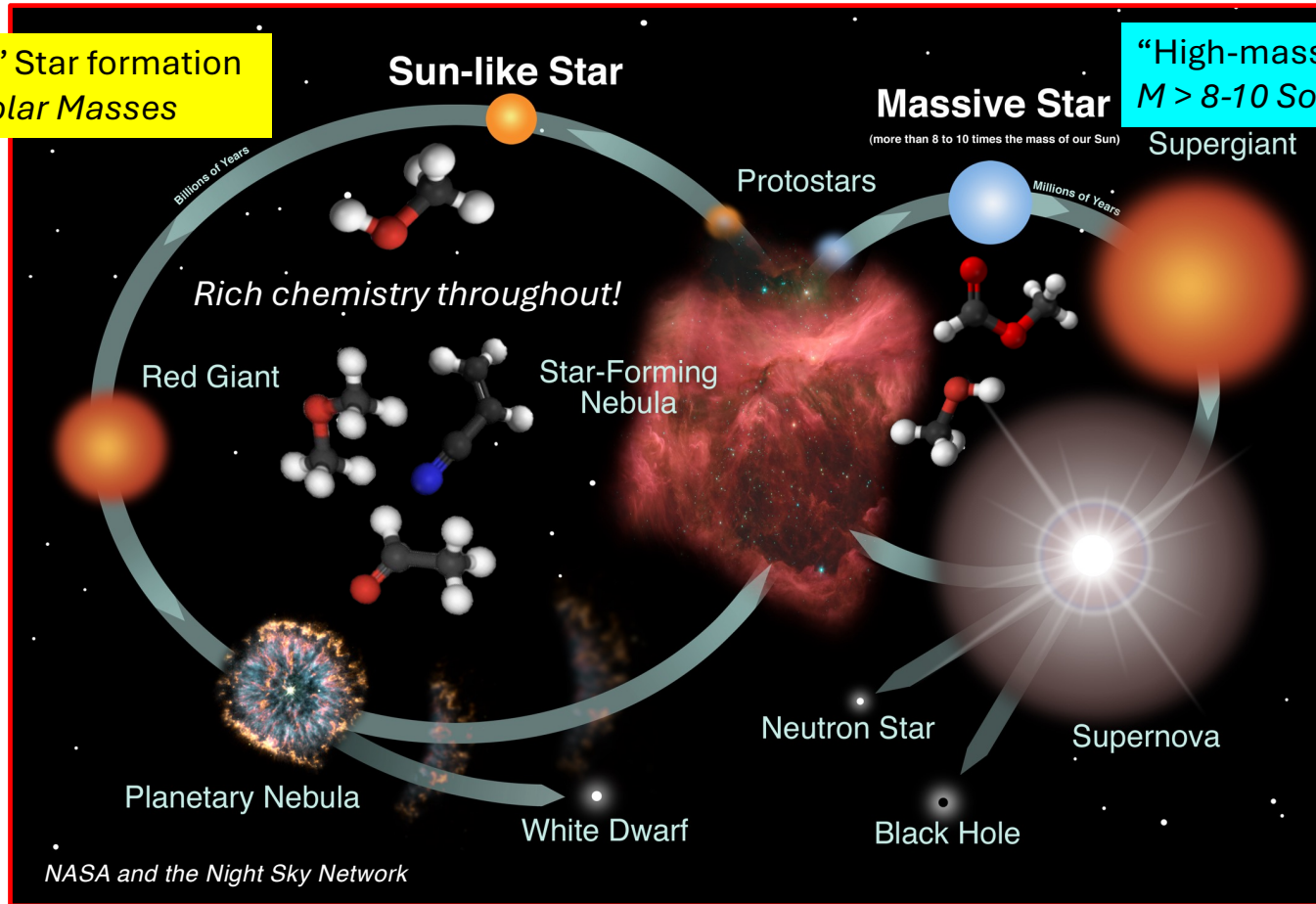
Credit: L. Ziurys

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“Low-mass” Star formation
 $M < \text{a few Solar Masses}$

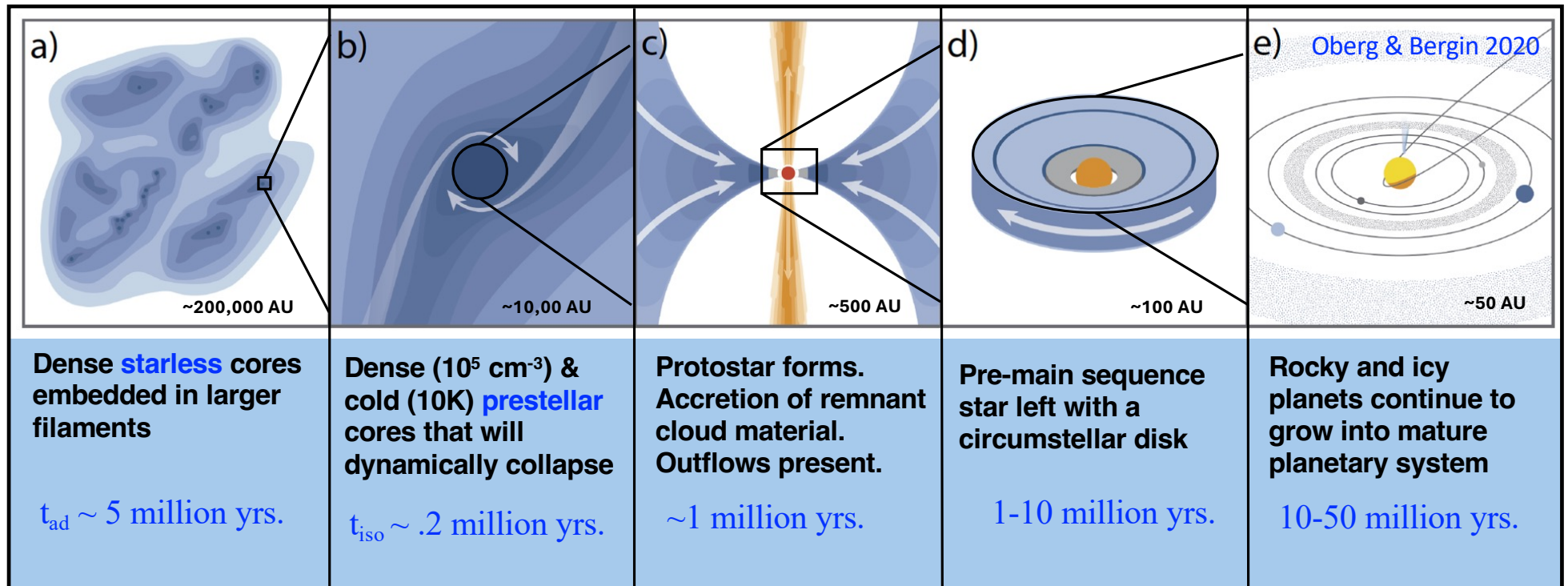
“High-mass” Star formation
 $M > 8-10 \text{ Solar Masses}$



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

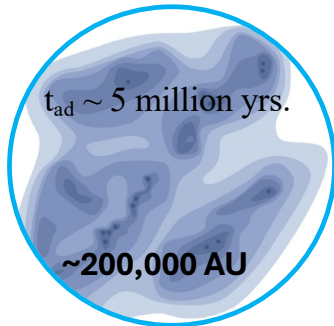


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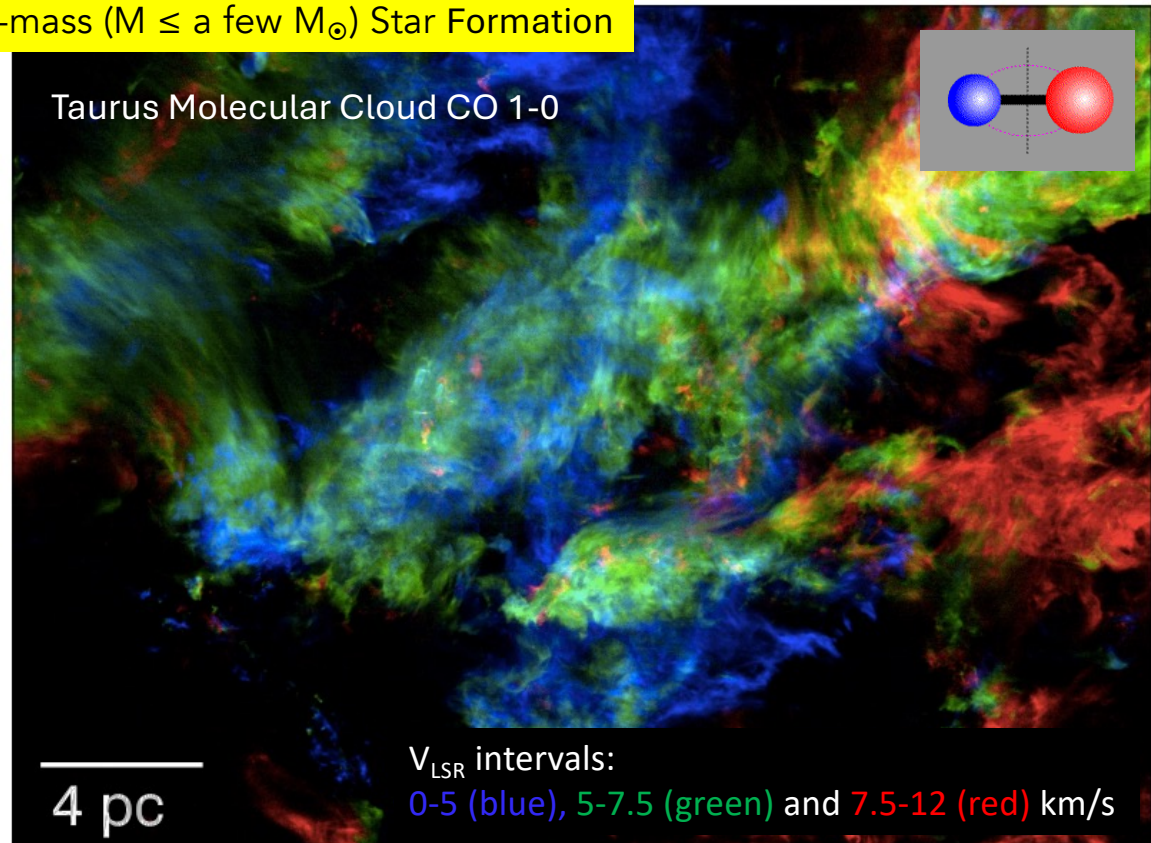


Molecular Line Data

Molecular clouds are comprised of molecular gas (mostly H_2 and CO) and dust which form filamentary structures



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

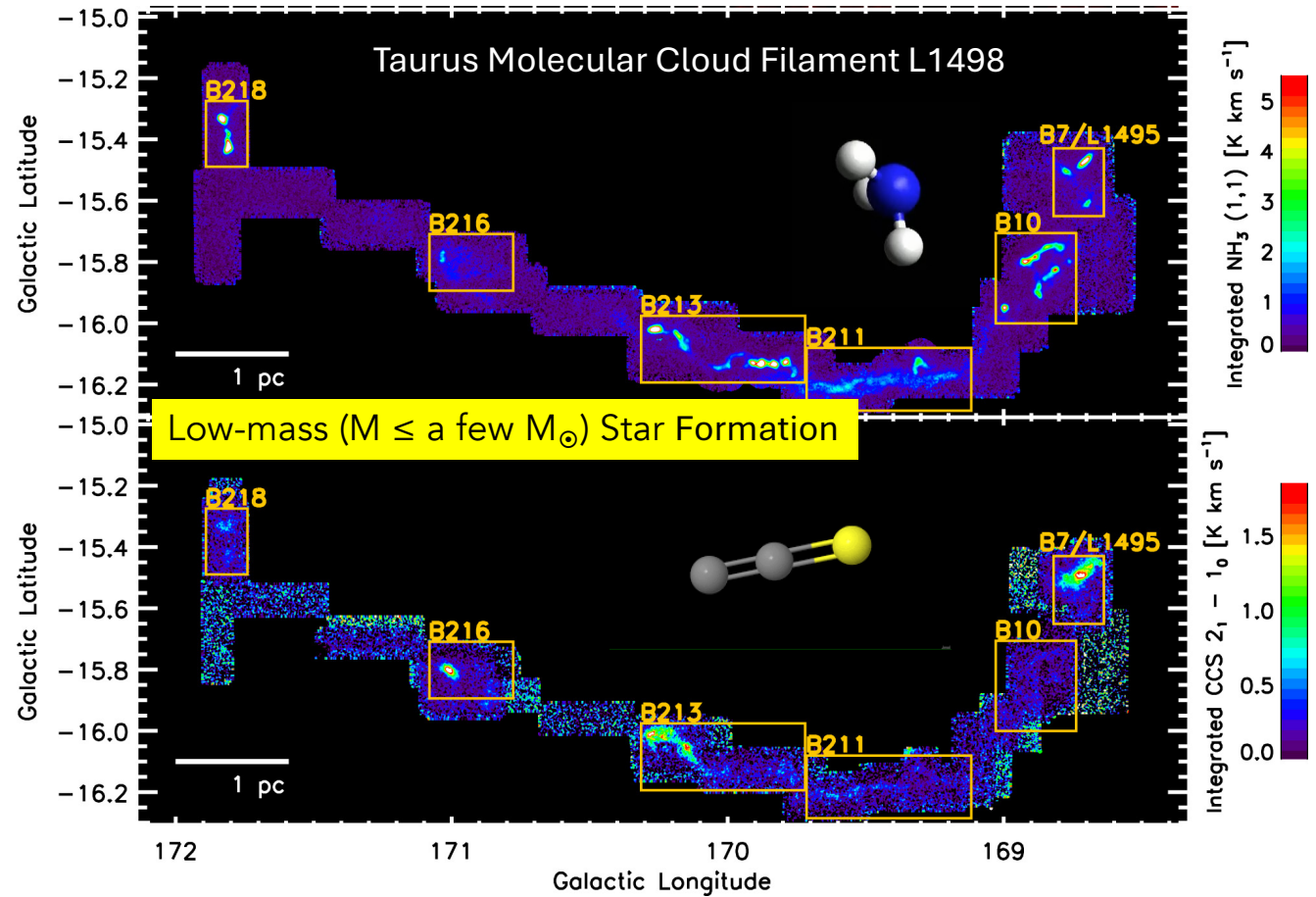
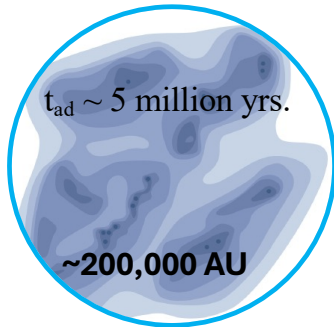


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Molecular Line Data

The filamentary structures are also traced by more 'exotic' molecular species, such as NH_3 and CCS

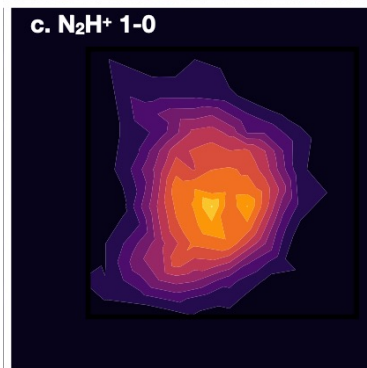
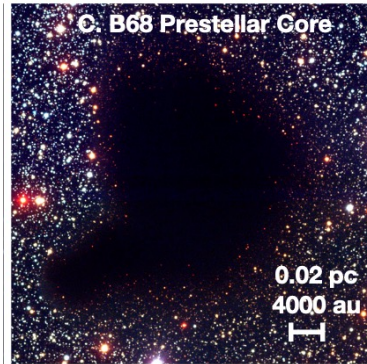
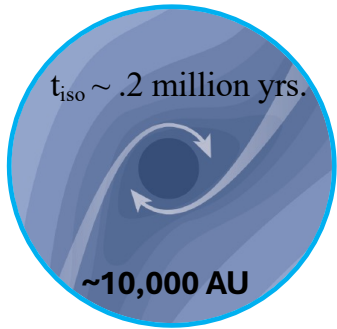


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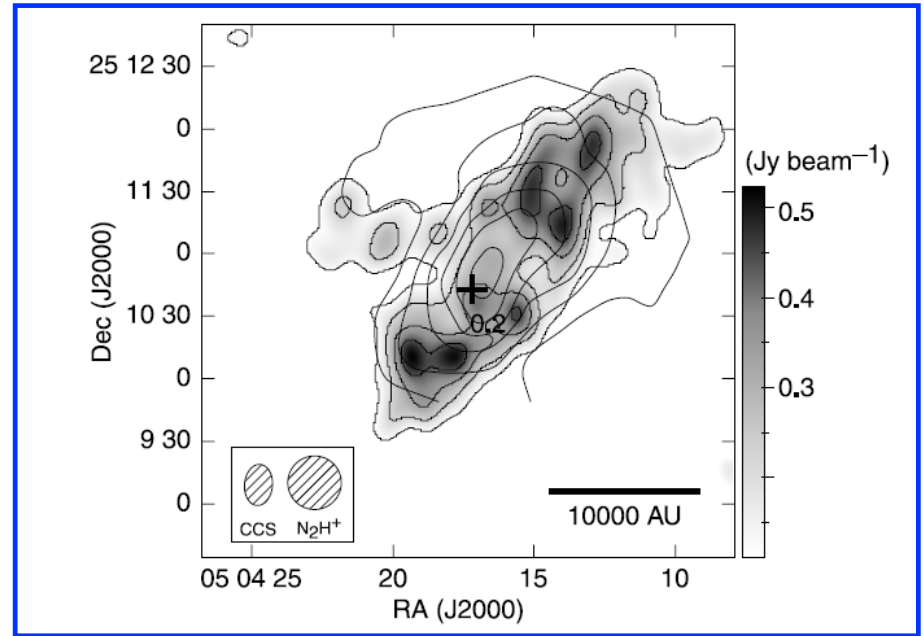
Molecular Line Data

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



Oberg & Bergin 2020

CCS (greyscale) \rightarrow freeze out towards denser and colder center
 N_2H^+ (contours) \rightarrow 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!

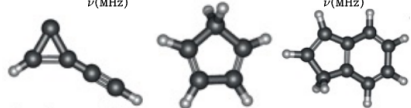
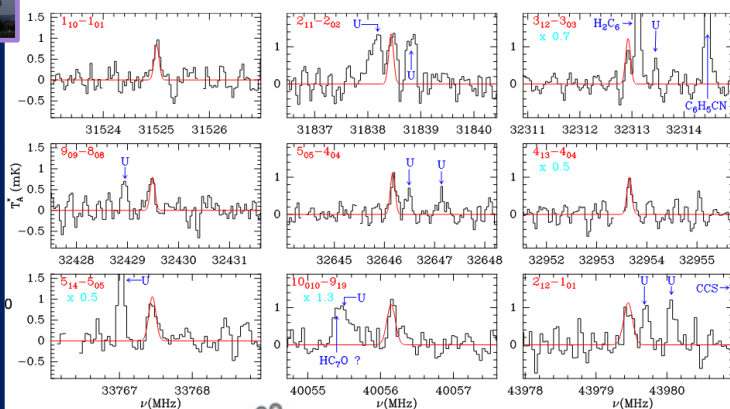


Yebes 40m Dish

TMC-1

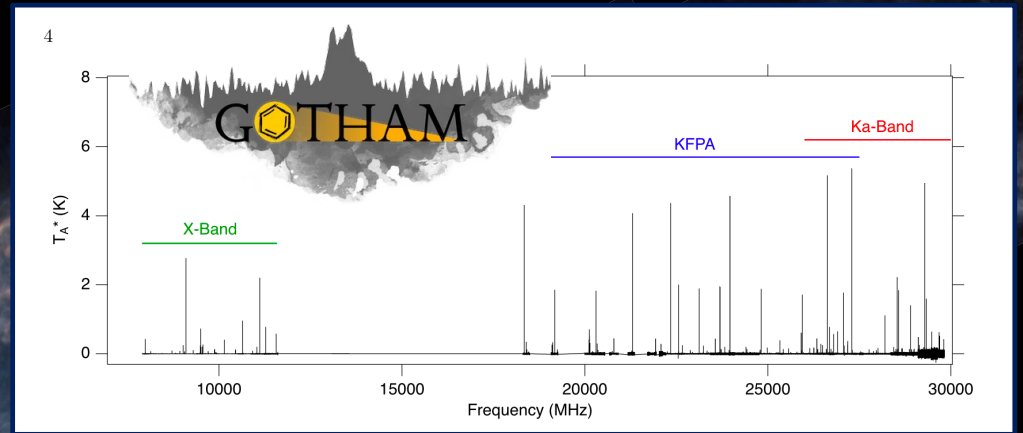


QUIJOTE Project (31-50 GHz)



+ Newly Discovered Hydrocarbon Chains and Cycles

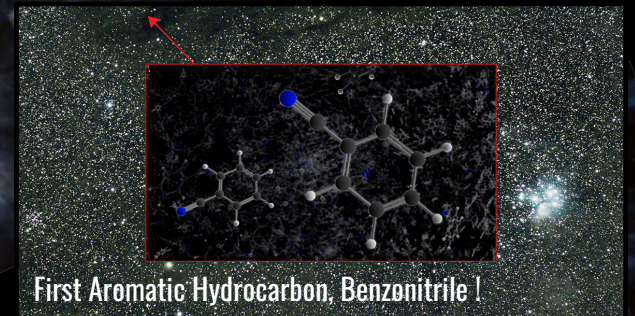
Cernicharo et al., 2021 & QUIJOTE team



McGuire et al. 2018, 2020



GBT 100m Dish

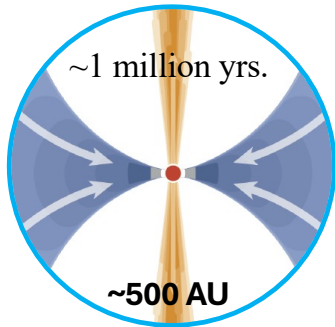


First Aromatic Hydrocarbon, Benzonitrile!

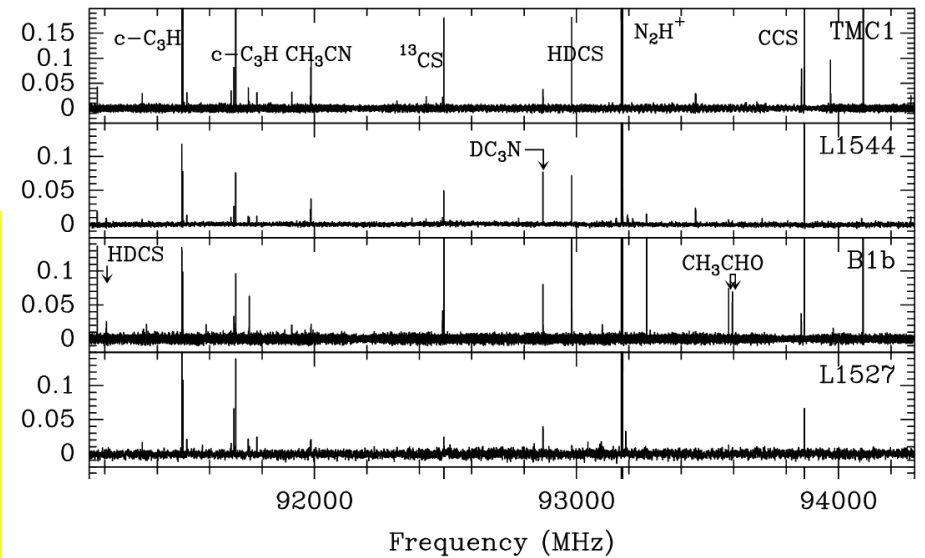
Blue 160 μ m, Green 250+350 μ m, Red 500 μ m
Credit: Herschel Gould Belt Team

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



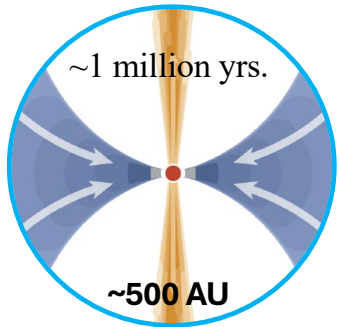
Lefloch et al., 2018

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Molecular Line Data

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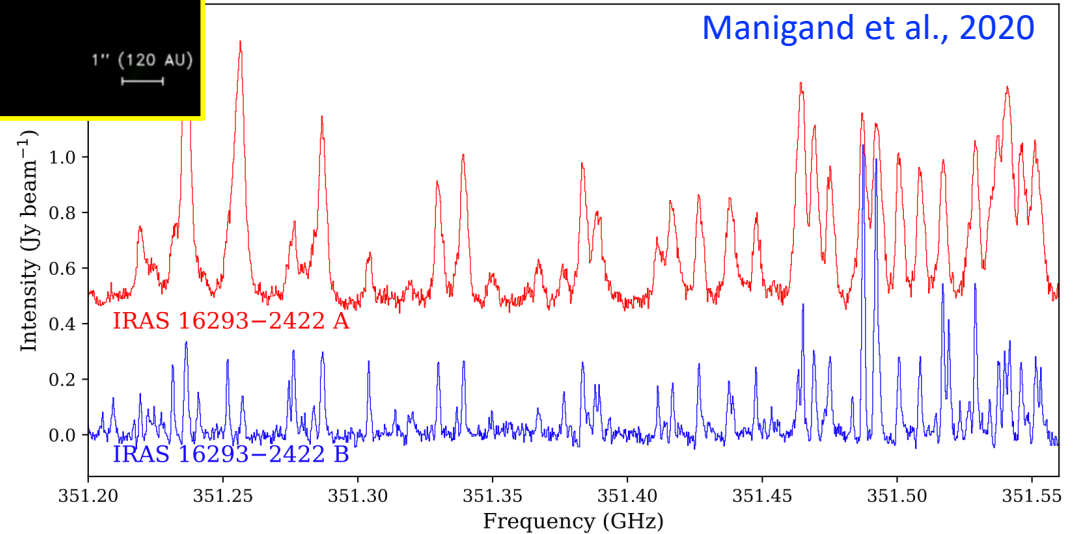


IRAS 16293-2422



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

Large program targeting many lines: ALMA PILS

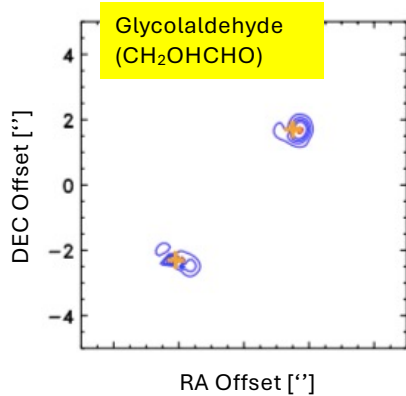
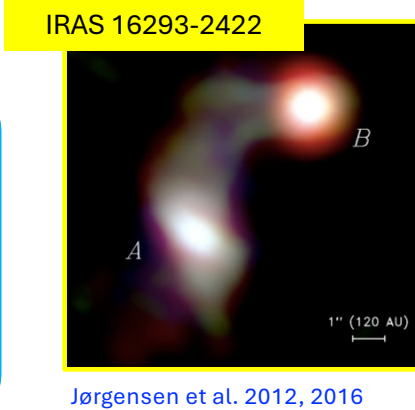
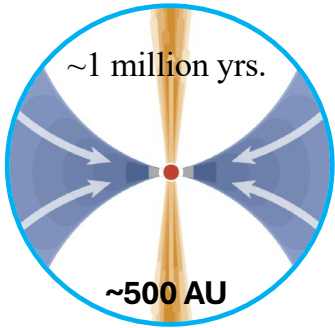


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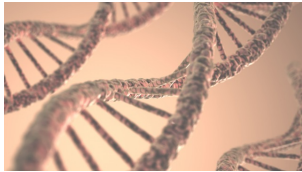


Molecular Line Data

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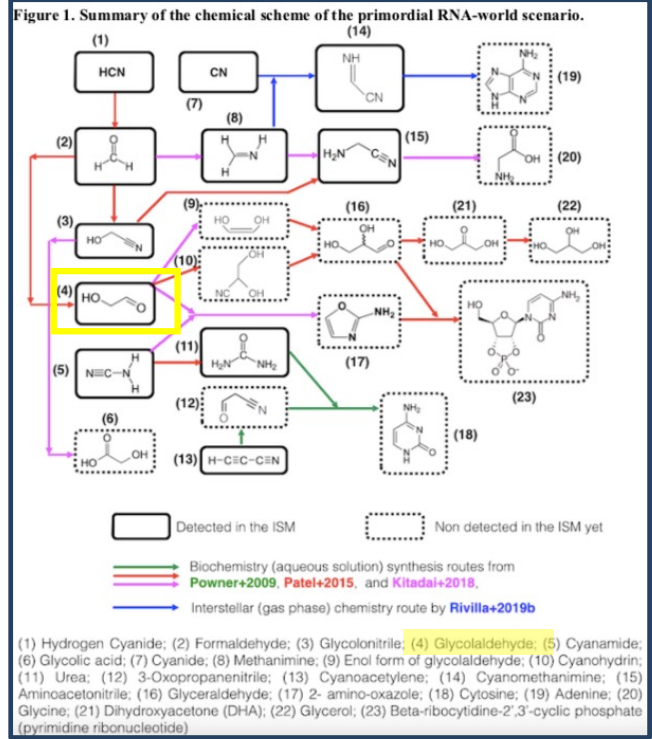


Low-mass ($M \leq$ a few M_{\odot}) Star Formation



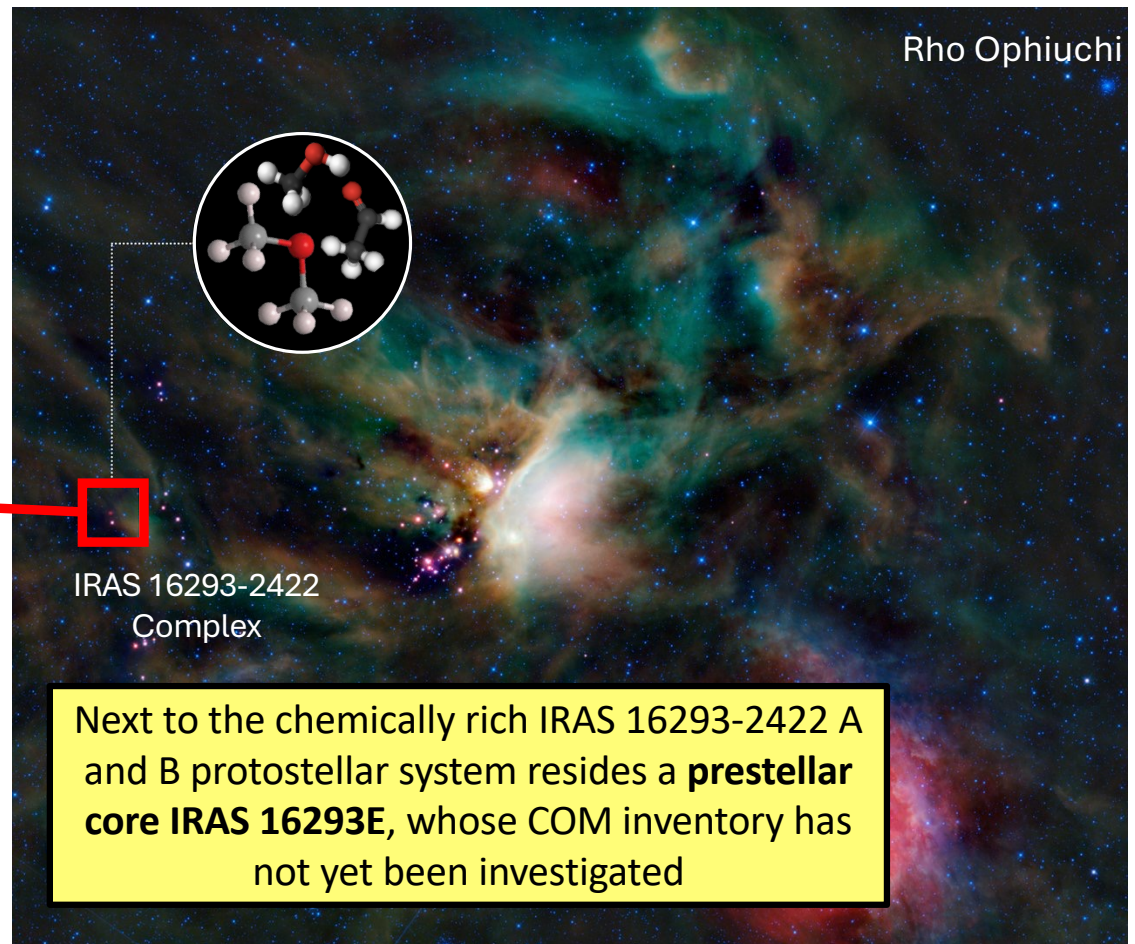
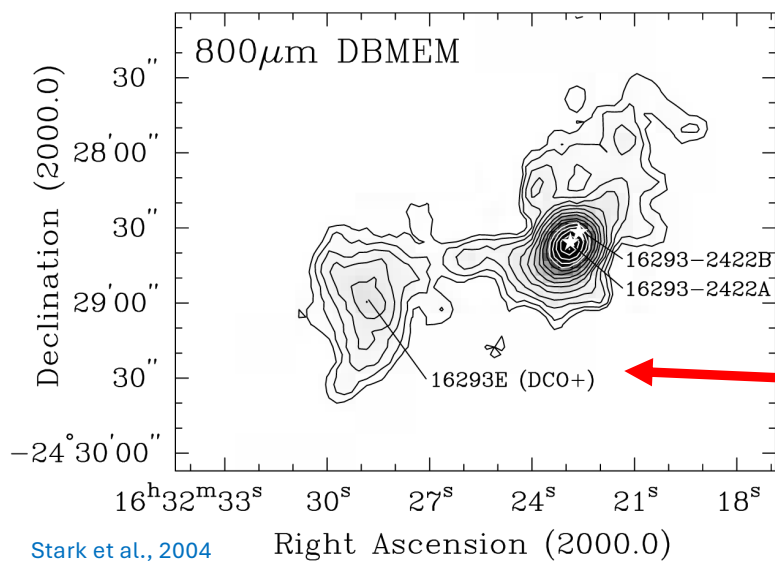
Life appeared on Earth about 4 billion years ago, but we do not know the processes that made it possible.

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.



Jimenez-Serra et al. 2020

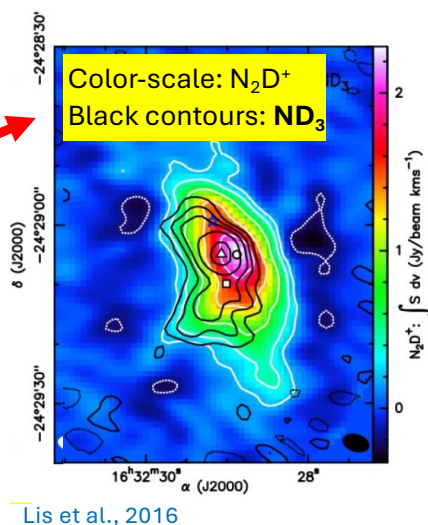
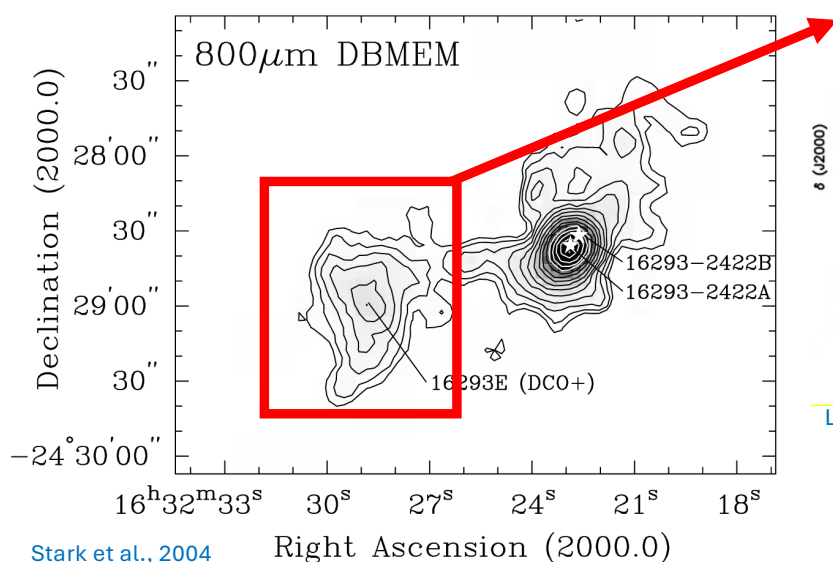
IRAS 16293E



Fractionation II, Florence, Italy, Nov 4th- 7th, 2024
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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 $D_2/D \sim 20\%$) compared to typical values in the ISM ($D/H \sim 10^{-5}$) 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!

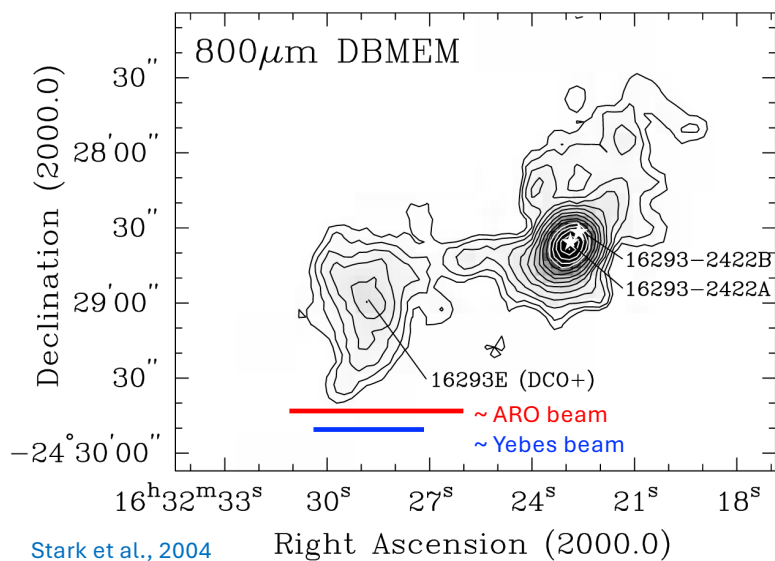
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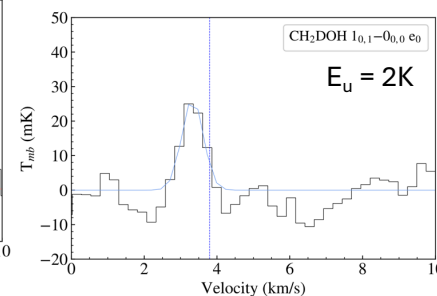
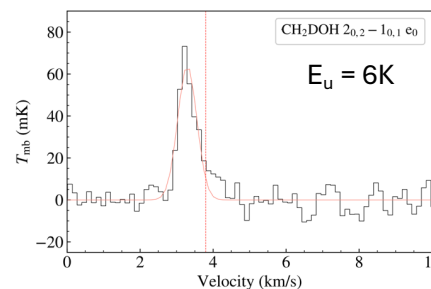
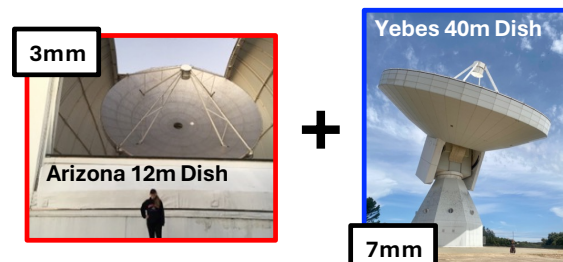


IRAS 16293E

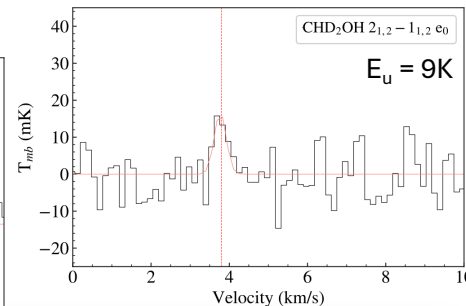
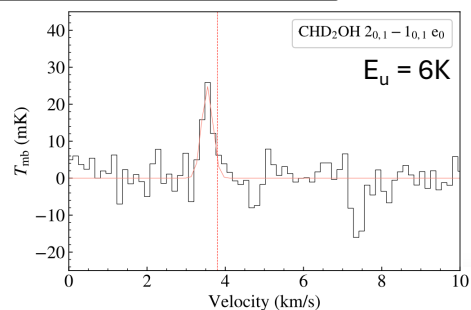


Single-pointed observations w/

Singly Deuterated Methanol!



Doubly Deuterated Methanol!



Scibelli et al., in prep

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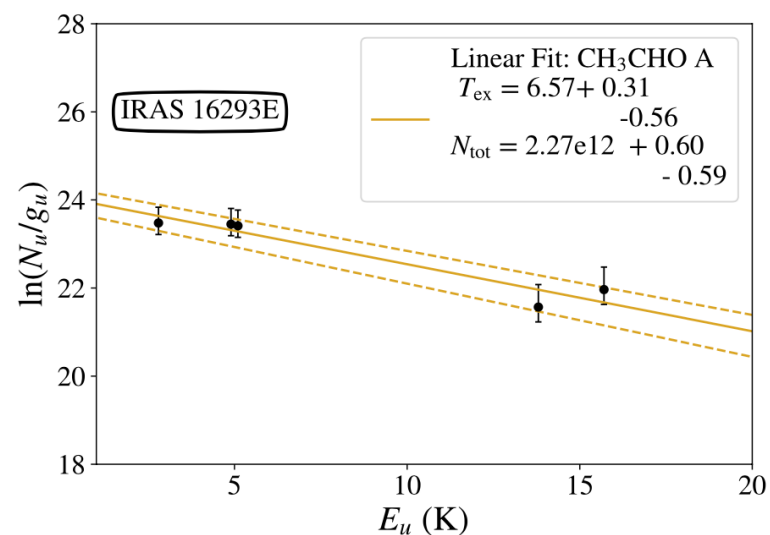
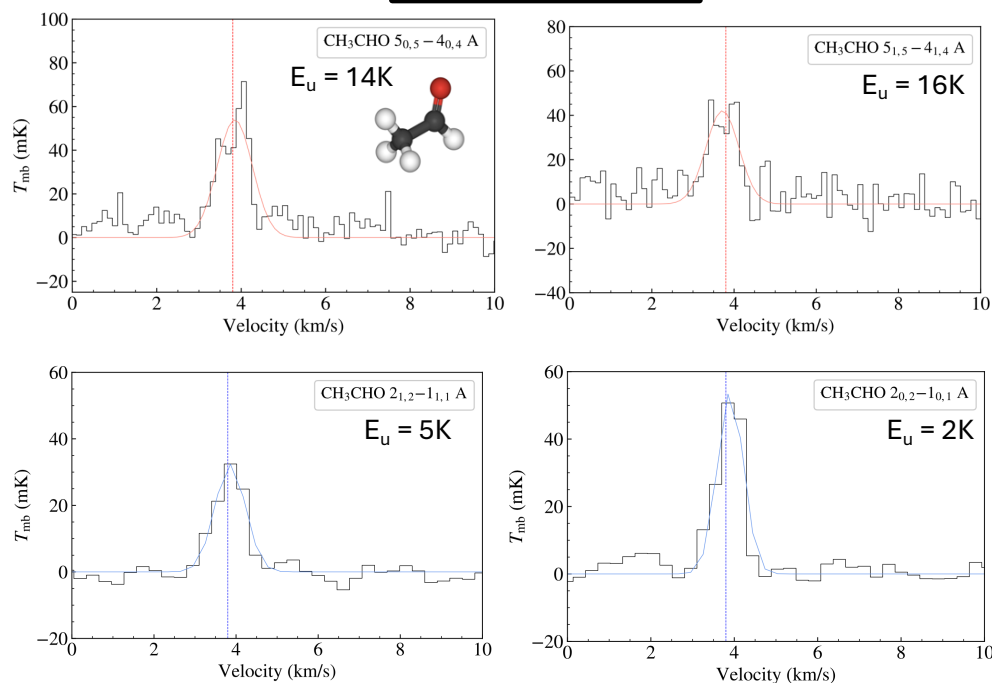
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IRAS 16293E

COM and dCOM column densities and excitation temperatures

Acetaldehyde



Scibelli et al., in prep

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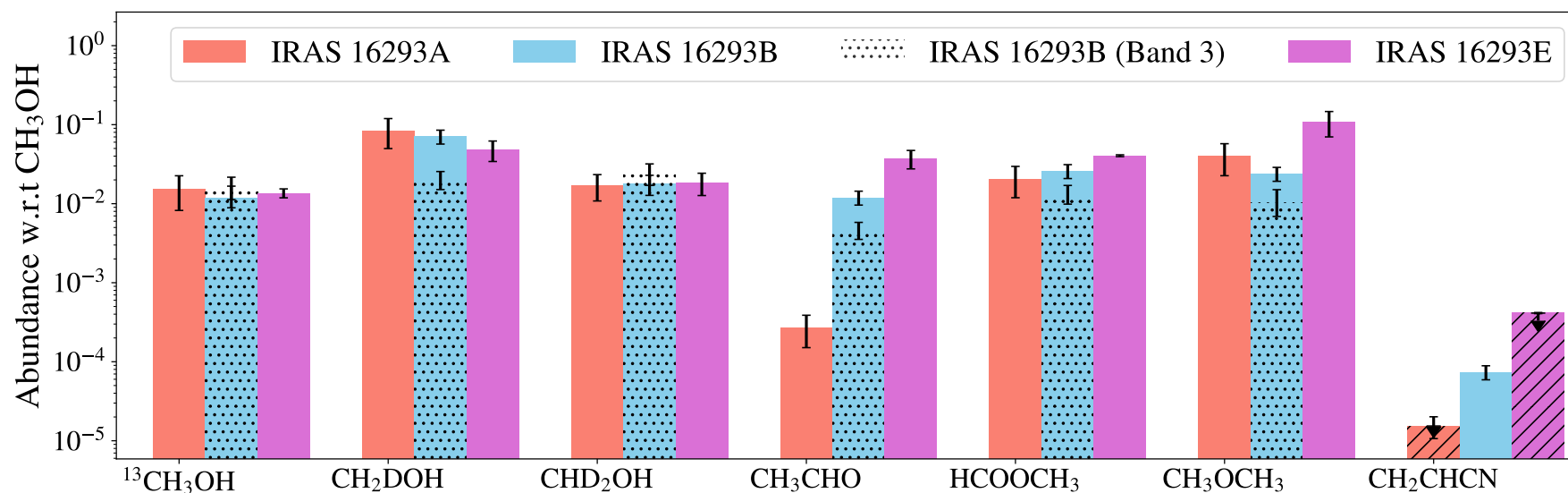
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IRAS 16293E

Striking similarity in abundances in IRAS 1293 A, B and E!
In particular, CHD₂OH 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

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Contact: sscibell@nrao.edu

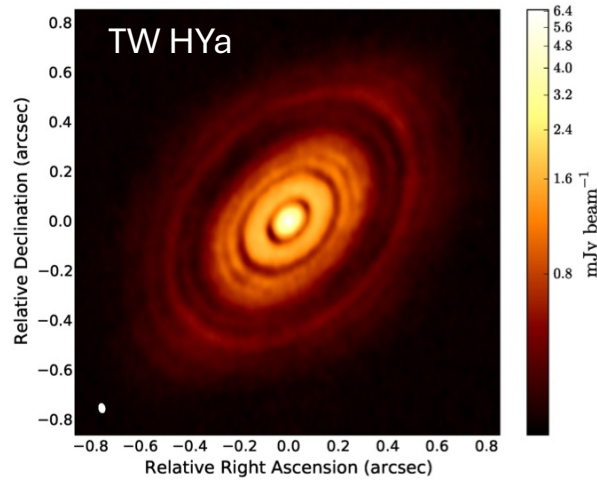
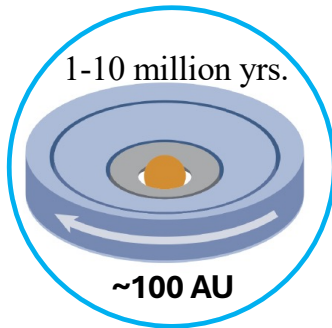


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Molecular Line Data

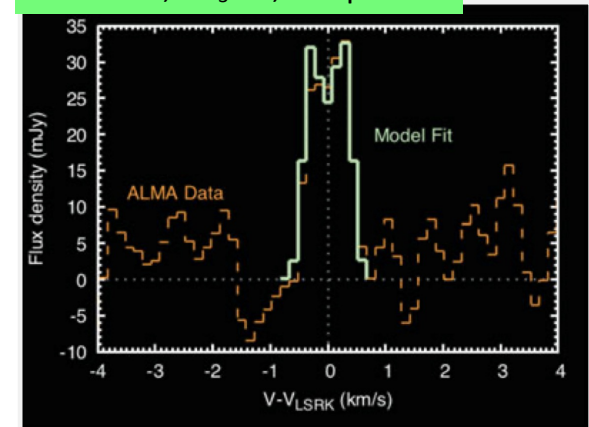
A protoplanetary disk show gaps in rings that signify planet formation!



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

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

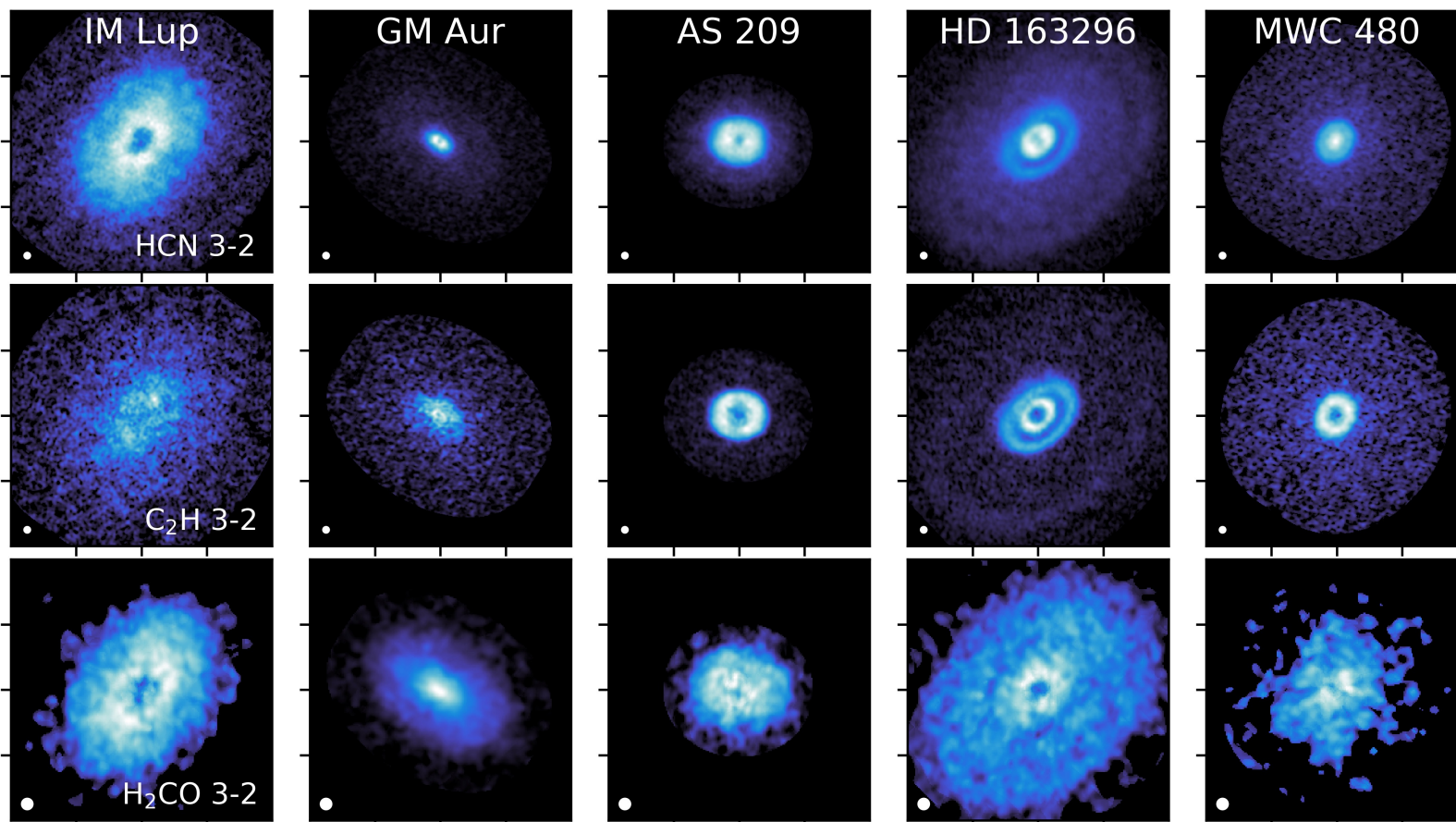
Methanol, CH₃OH, line profile



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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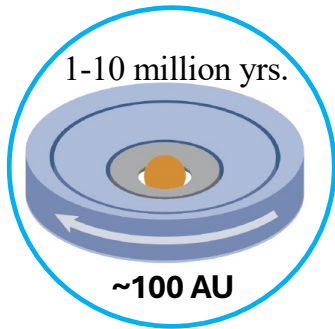


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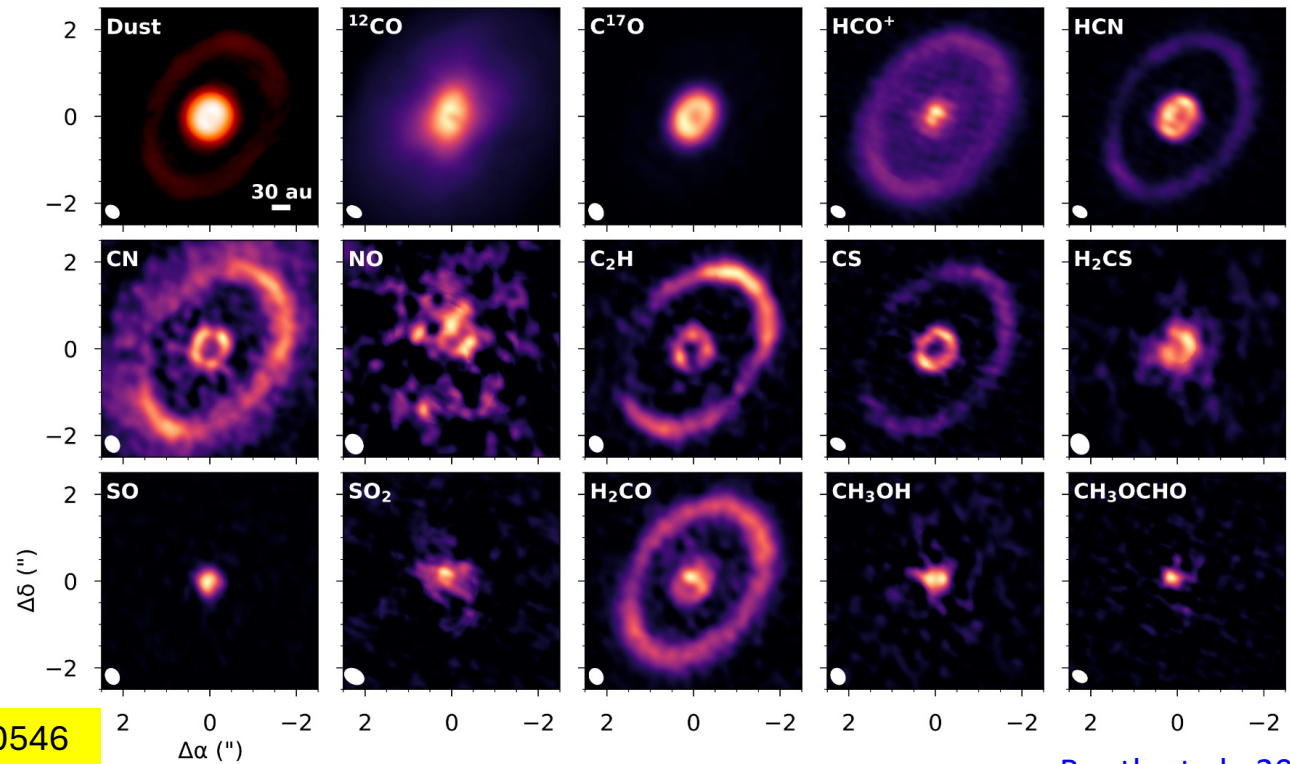


Molecular Line Data

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



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



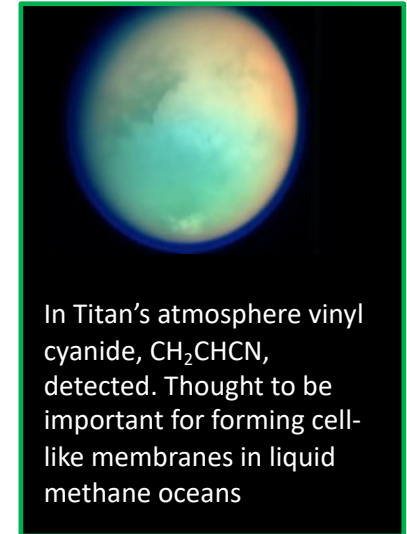
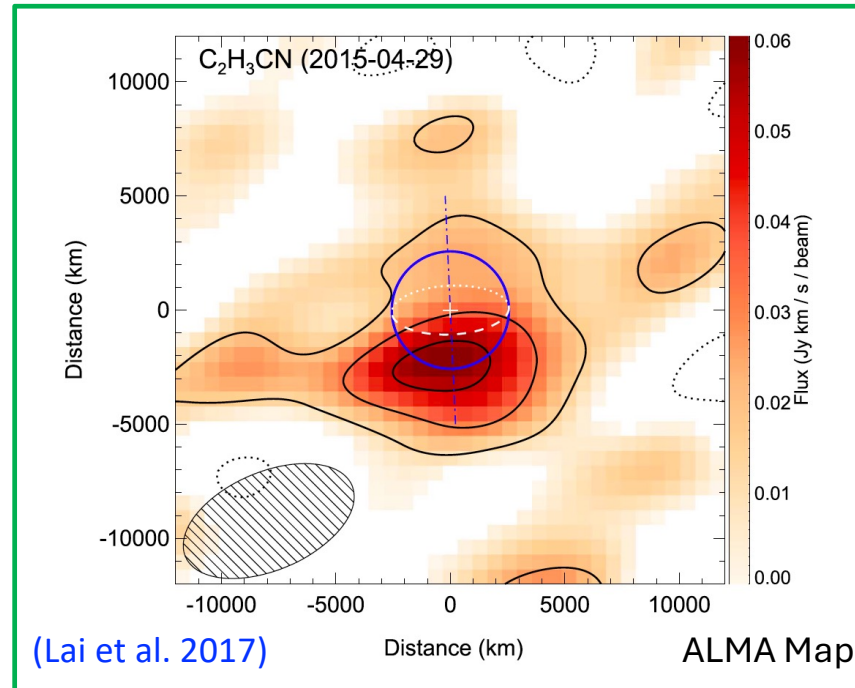
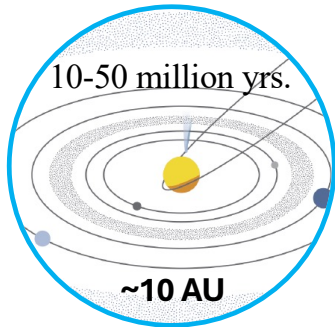
Booth et al., 2024a

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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*

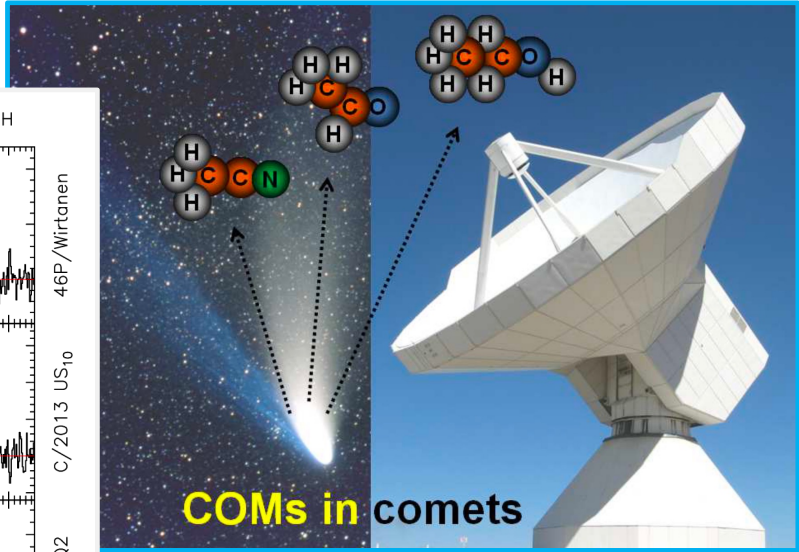
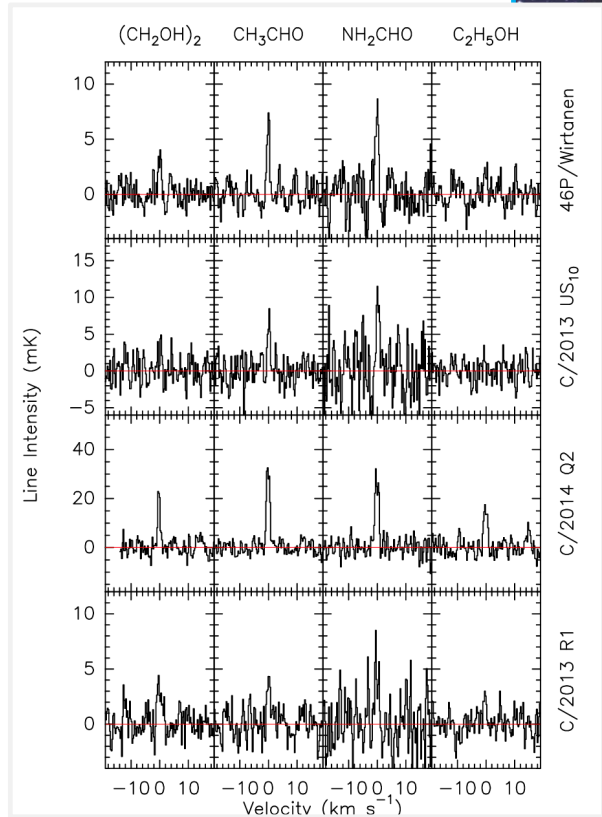
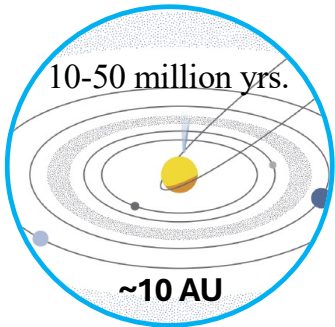


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Molecular Line Data

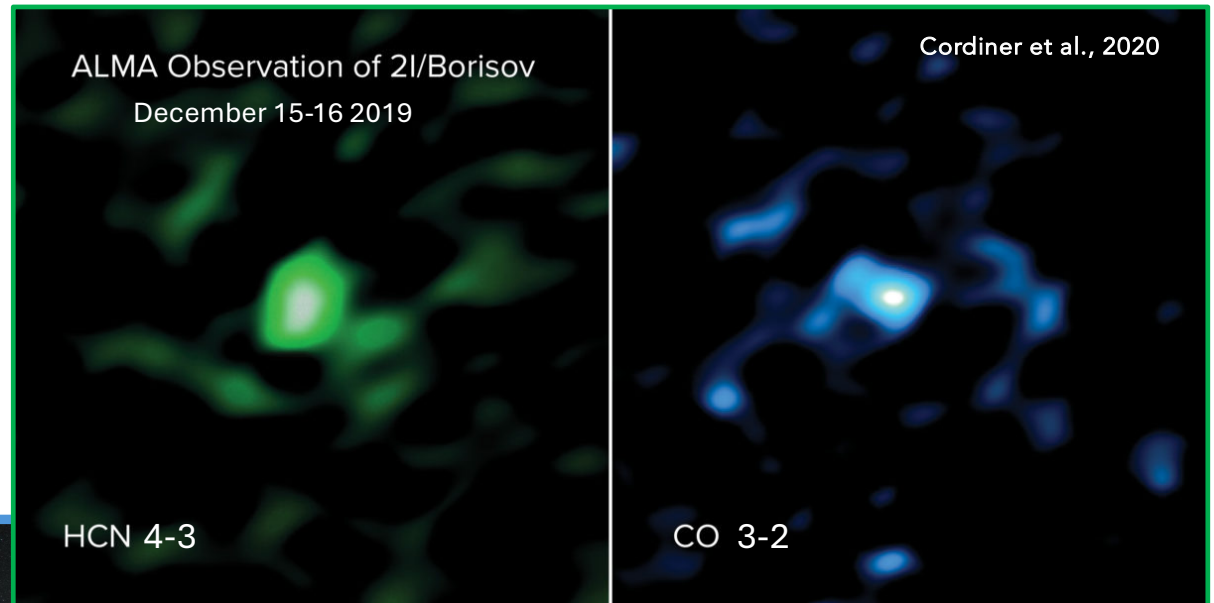
Rocky and icy planets and moons, as well as planetesimals (e.g., asteroids, comets), continue to grow into a mature *planetary system*



Biver 2019

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)



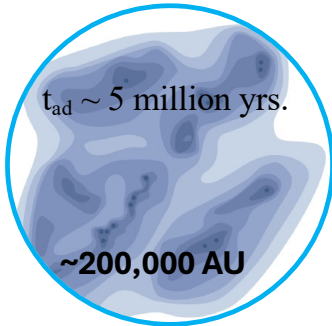
Maps from rotational line spectra

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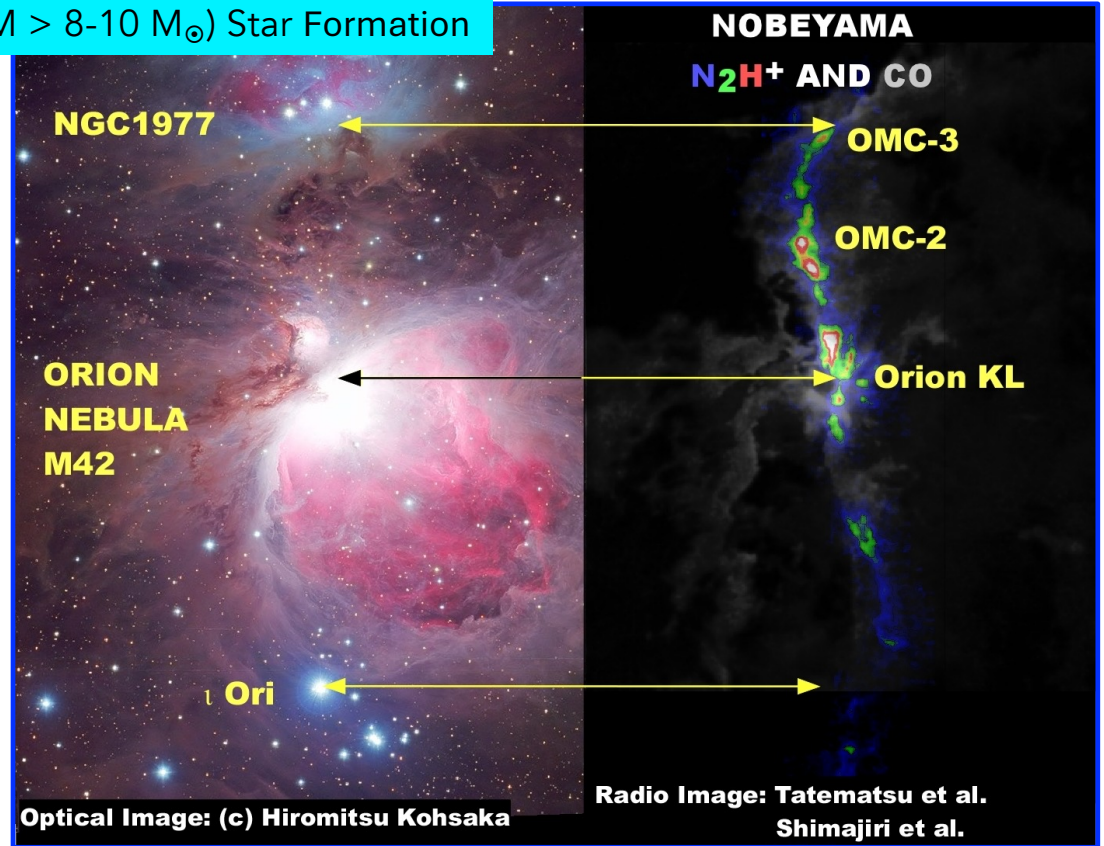


Molecular Line Data

Molecular clouds are comprised of molecular gas (mostly H₂ and CO) and dust which form filamentary structures



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

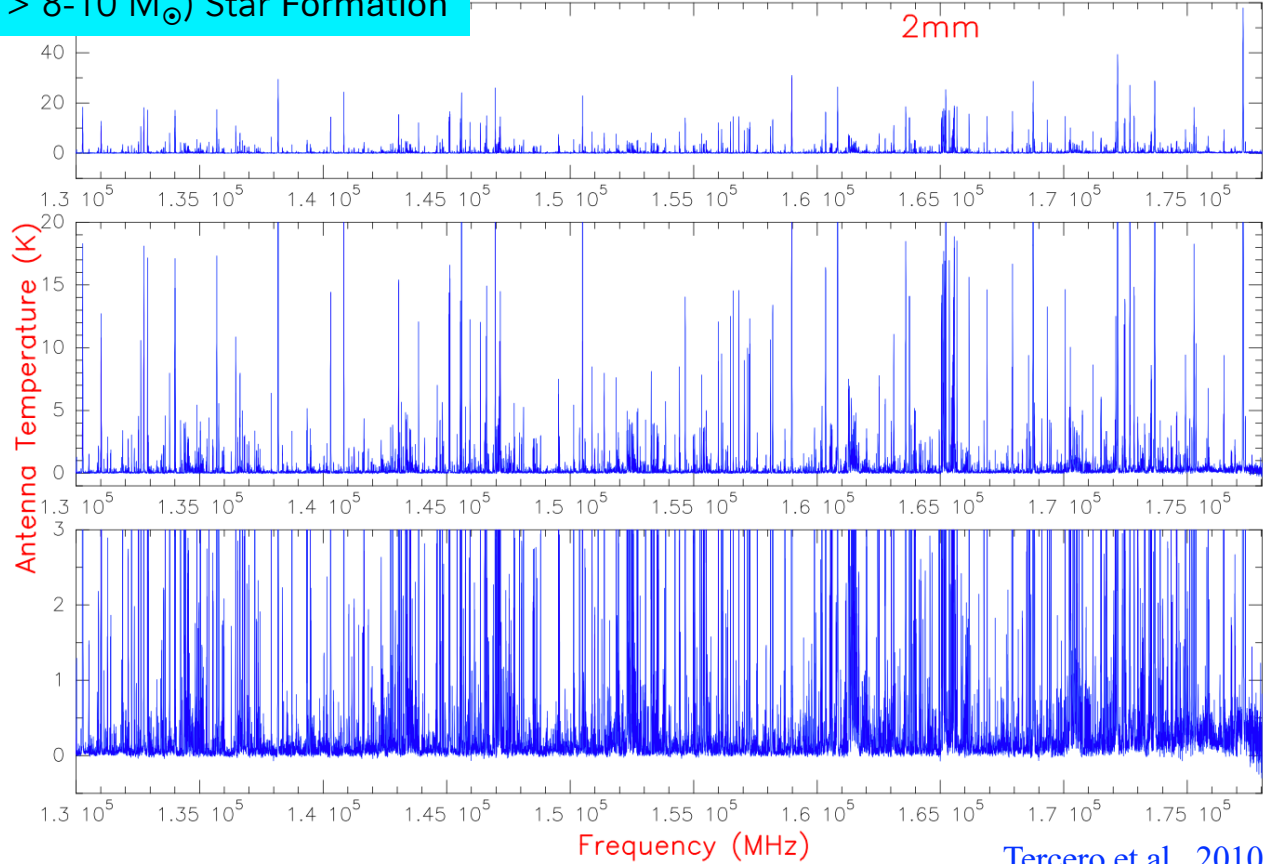


<https://www.nro.nao.ac.jp/~kt/html/kt-e.html>

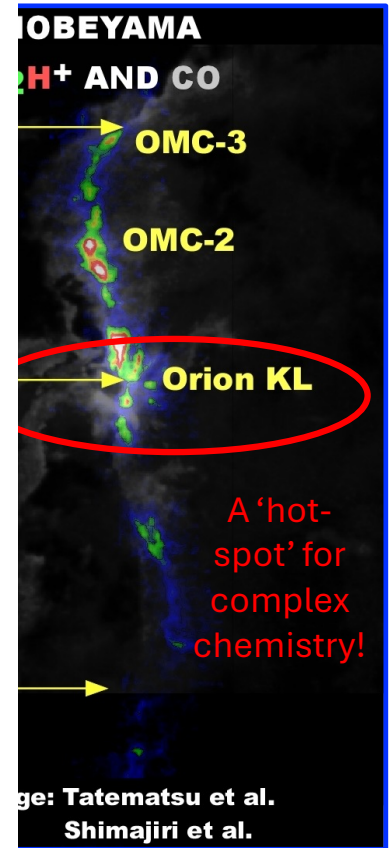
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High-mass ($M > 8-10 M_{\odot}$) Star Formation



Tercero et al., 2010

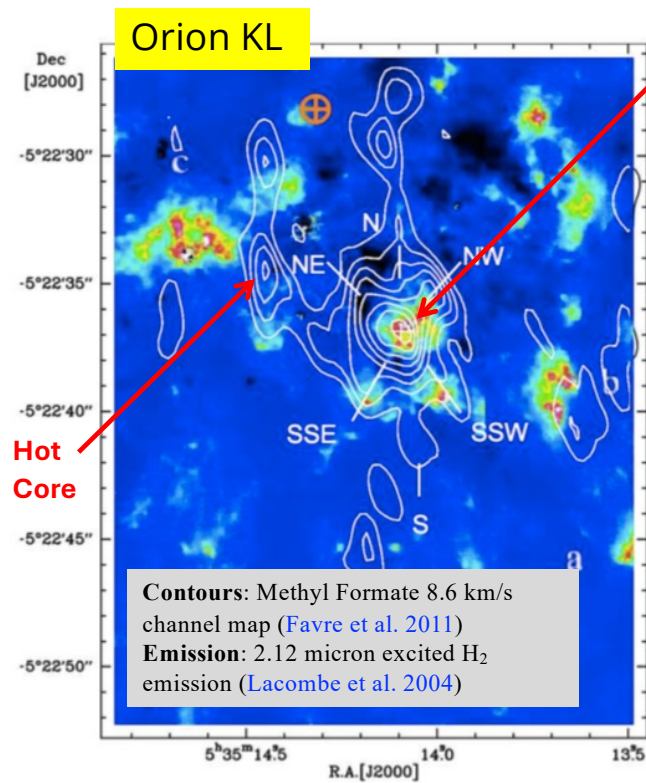


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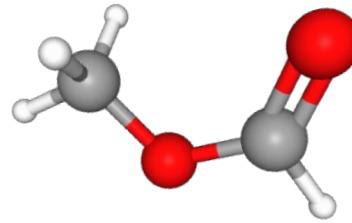


Molecular Line Data

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

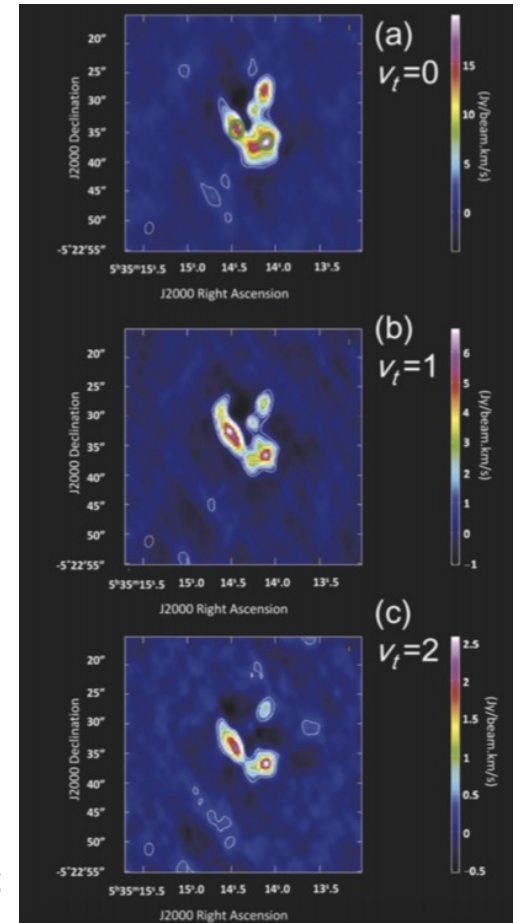


8-atom molecule, Methyl Formate, HCOOCH₃, tracing the star-forming 'hot core'



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

Sakai et al. 2015

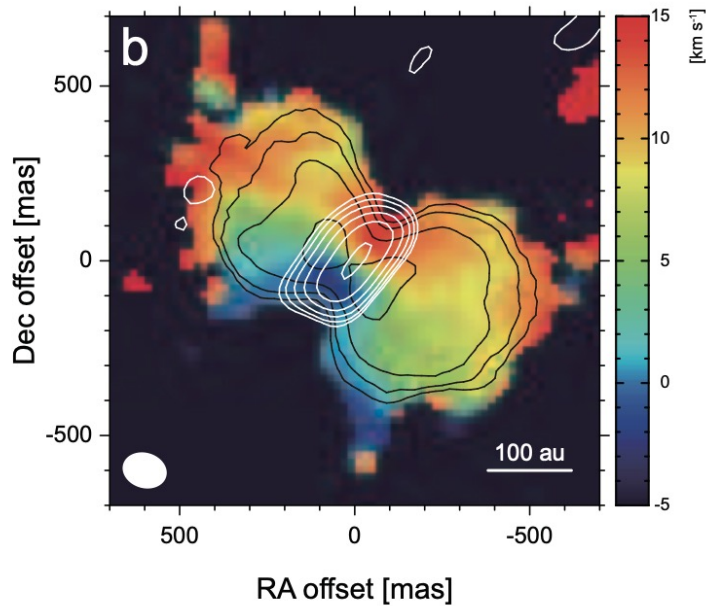


Molecular Line Data

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

Orion Source I

SiO emission



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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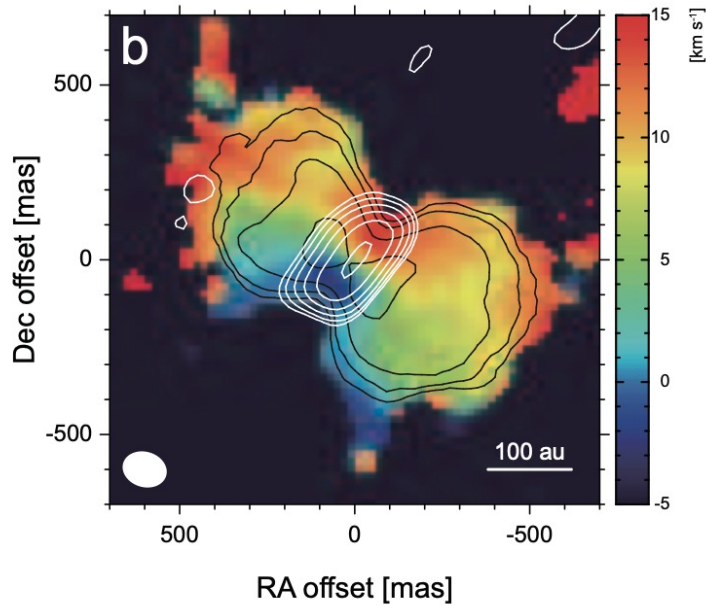


Molecular Line Data

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

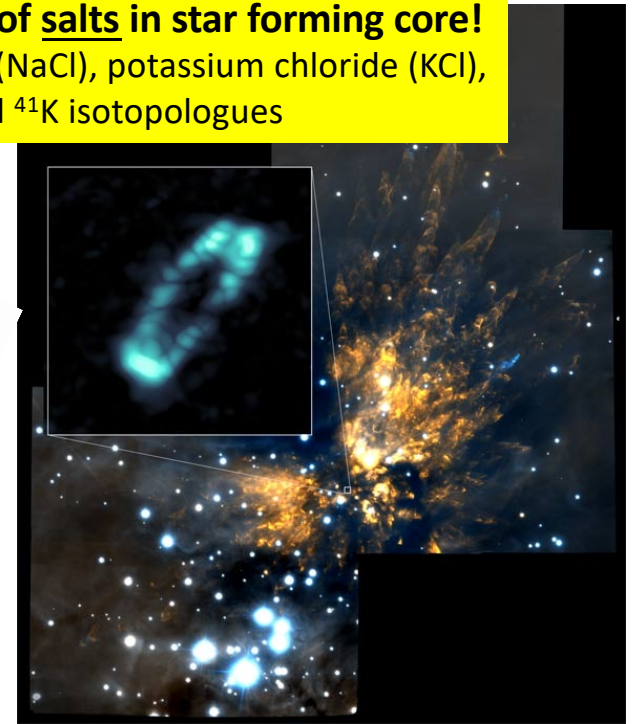
Orion Source I

SiO emission



First detection of salts in star forming core!

Sodium chloride (NaCl), potassium chloride (KCl), and their ^{37}Cl and ^{41}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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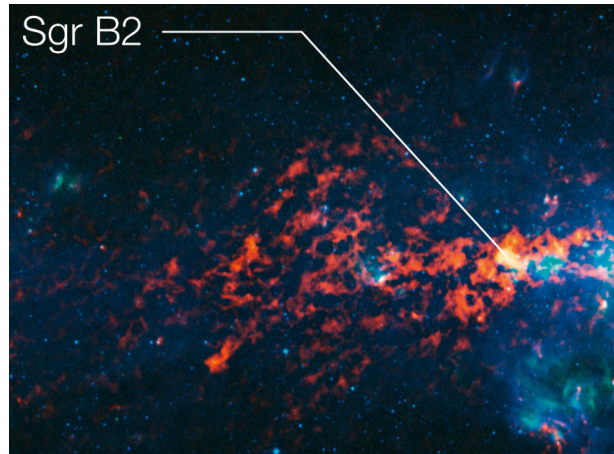


Molecular Line Data

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

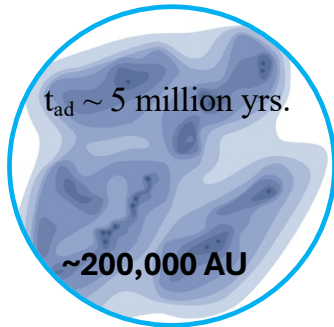
of molecule discoveries per source

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



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

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



McGuire 2022

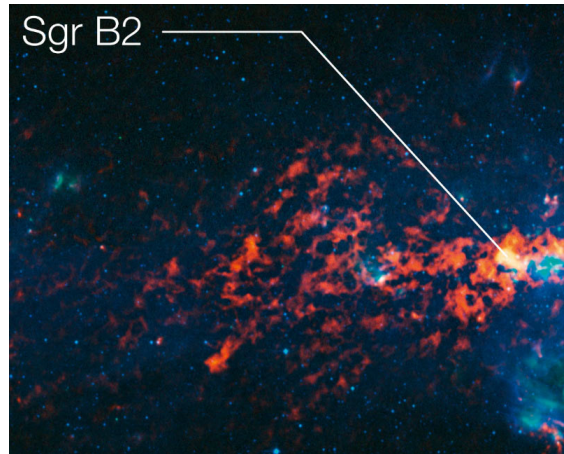
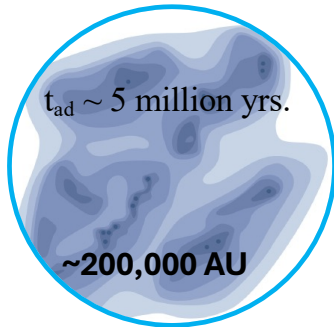
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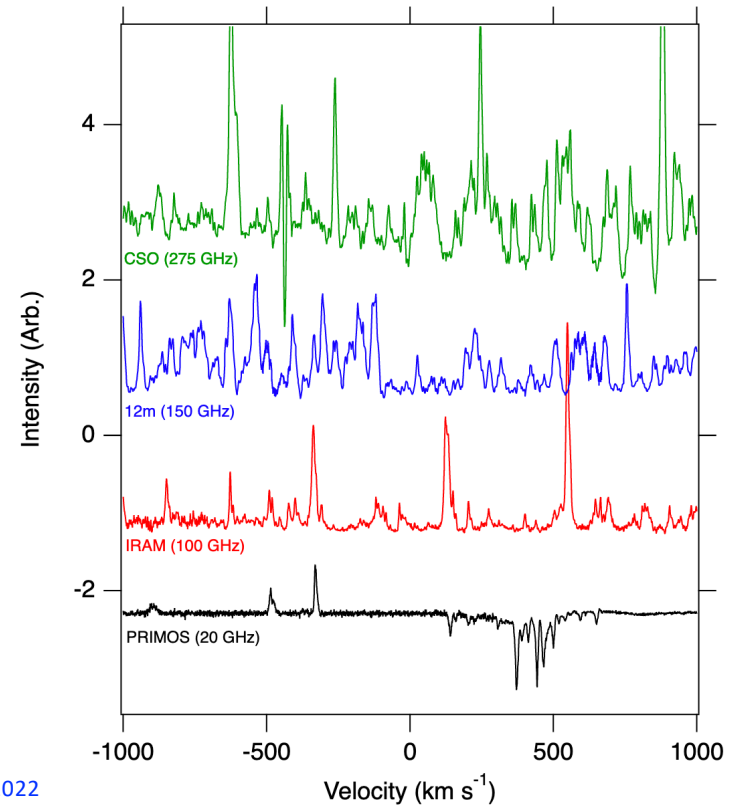
Molecular Line Data

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
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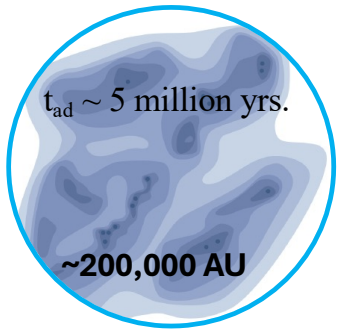
McGuire 2022

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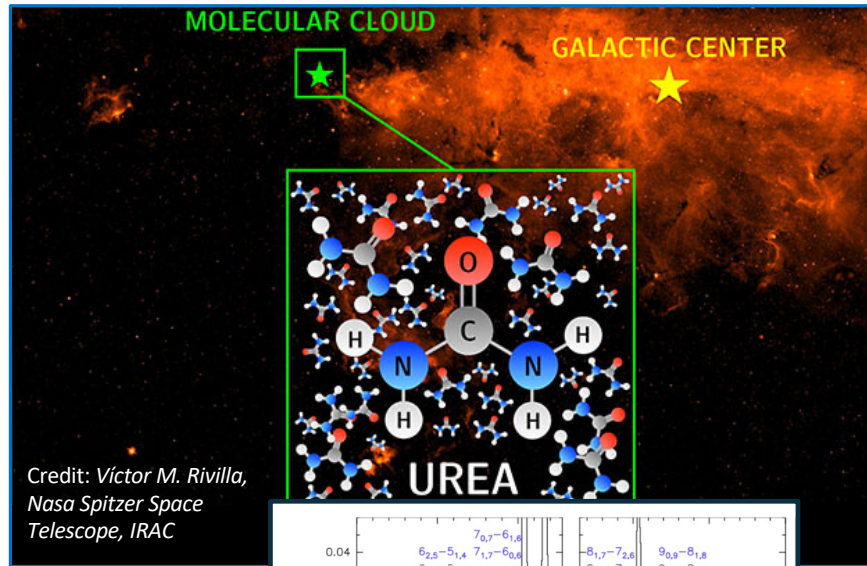
Molecular Line Data

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

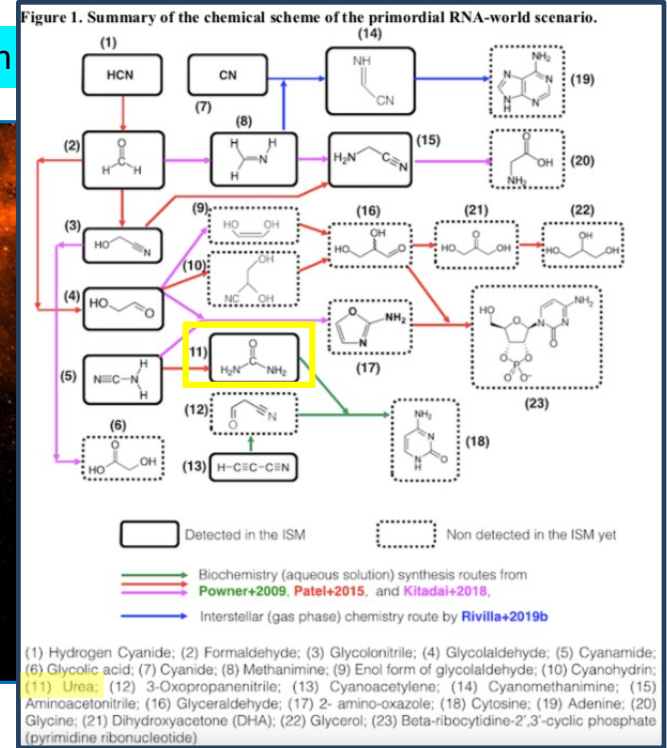
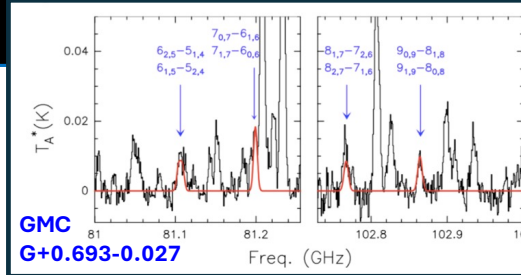


Recent Detections of biologically relevant molecule UREA (NH_2CONH_2)

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



Credit: *Victor M. Rivilla, Nasa Spitzer Space Telescope, IRAC*



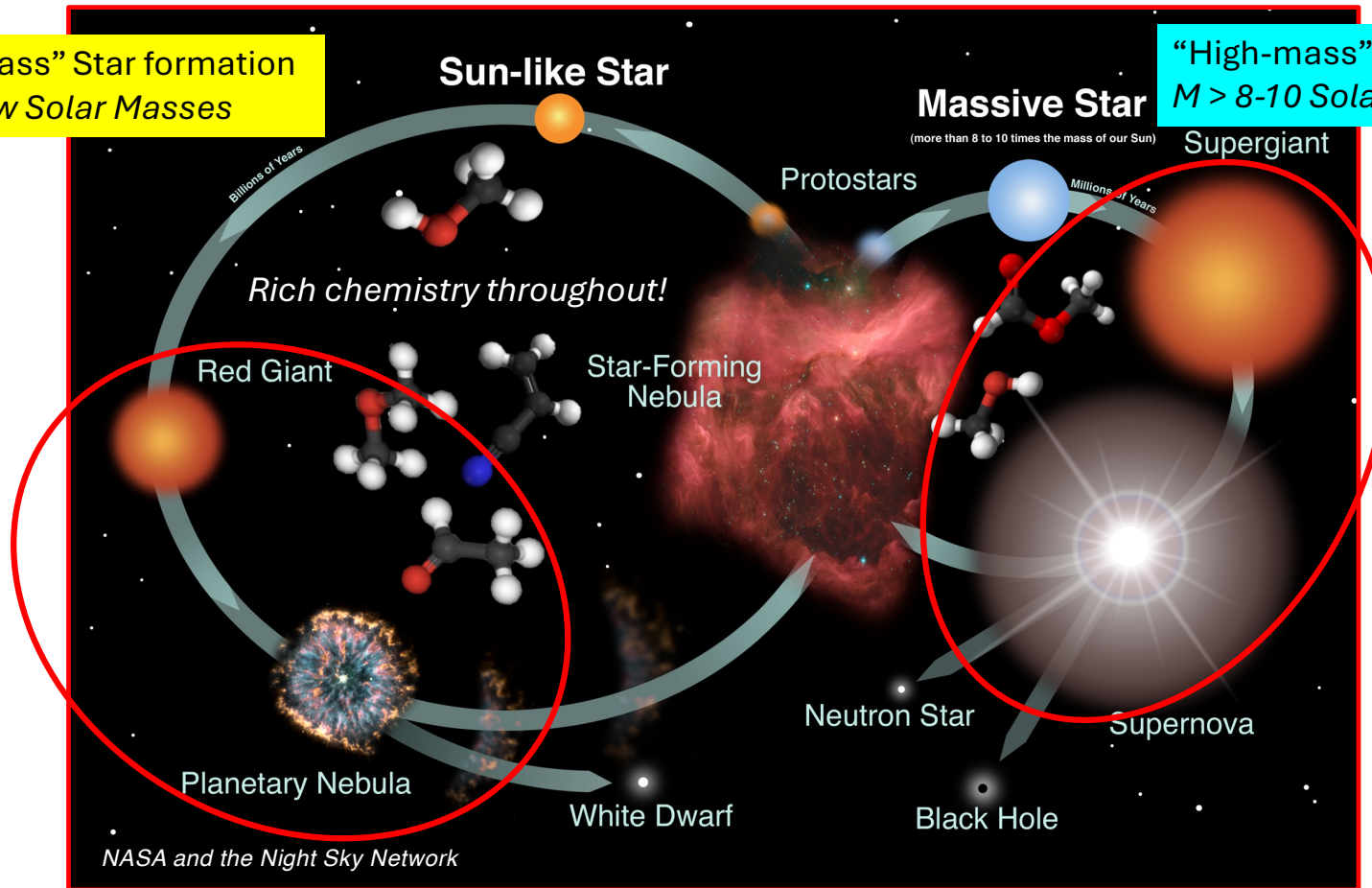
Jiménez-Serra et al. 2020

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“Low-mass” Star formation
 $M < \text{a few Solar Masses}$

“High-mass” Star formation
 $M > 8-10 \text{ Solar Masses}$

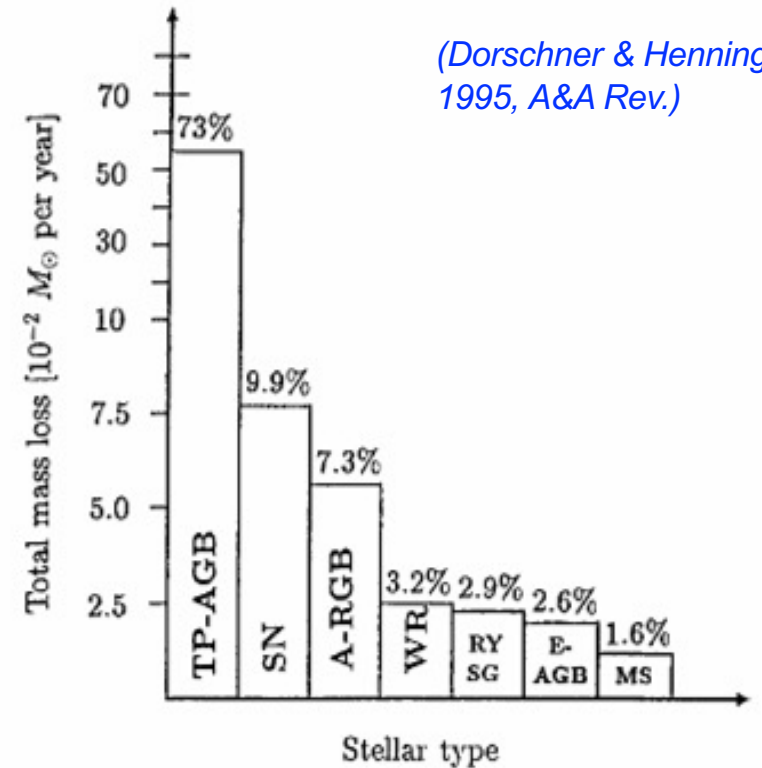


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EVOLVED STARS

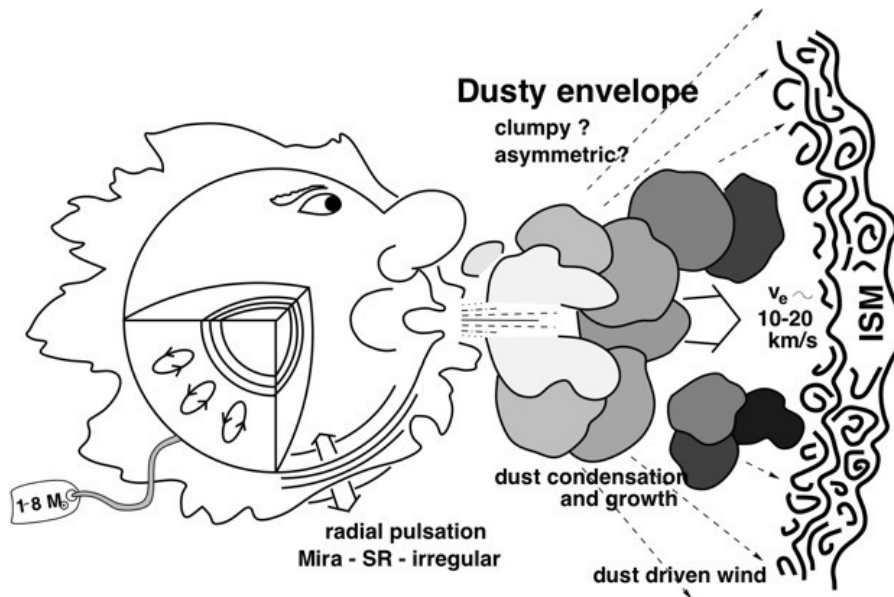
- **IMPORTANT** in astrochemistry because material is cycled back to the ISM!
- Mass loss from evolved stars
 - ⇒ **Supplies 85% of material in ISM**
- Material cycled in **circumstellar shells of low-mass giants**
- Remainder from **Supernovae and Wolf-Rayet Stars**
- Material ends up in diffuse clouds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



Credit: L. Ziurys

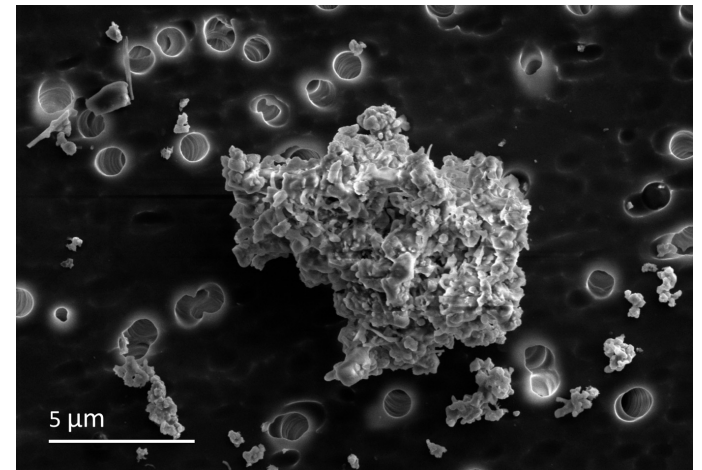
Molecular Line Data

Asymptotic Giant Branch (AGB) Stars



Olofsson 2011

Dust Grains born from material ejected from stars!



Credit: Hope Ishii, University of Hawai'i.

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

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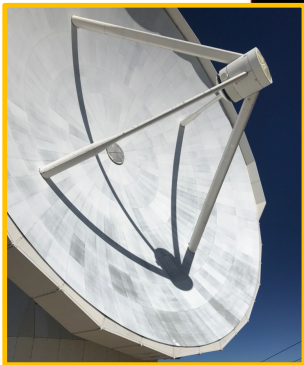


Molecular Line Data

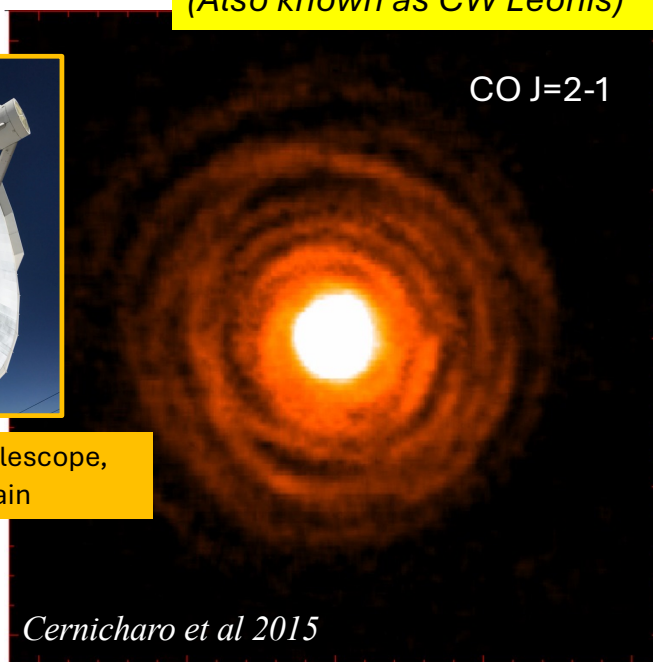
Asymptotic Giant Branch (AGB) Stars

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

(Also known as CW Leonis)



IRAM 30m Radio Telescope,
Granada, Spain



Cernicharo et al 2015

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
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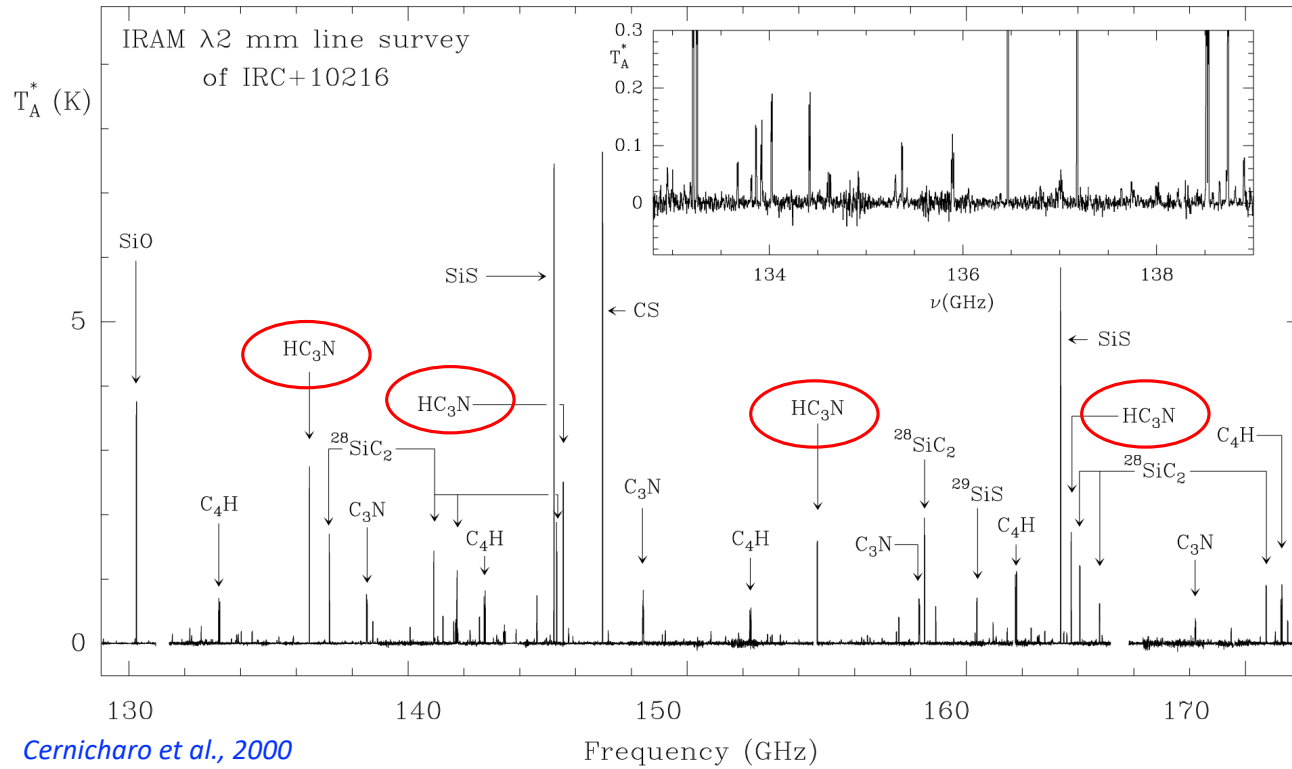
McGuire 2022

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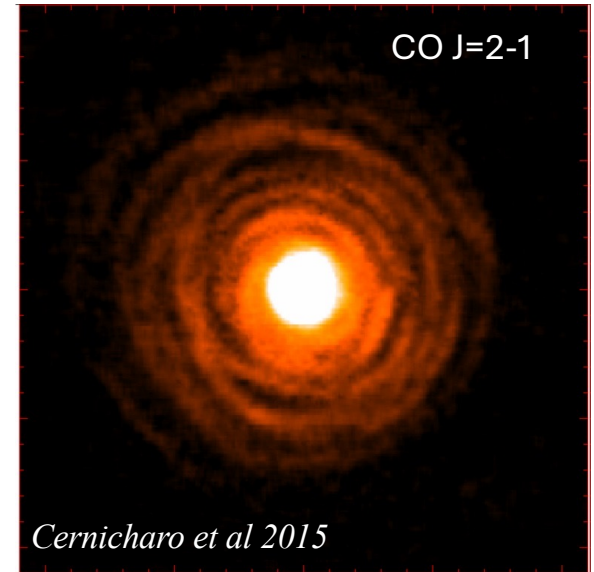


Molecular Line Data

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



Cernicharo et al., 2000

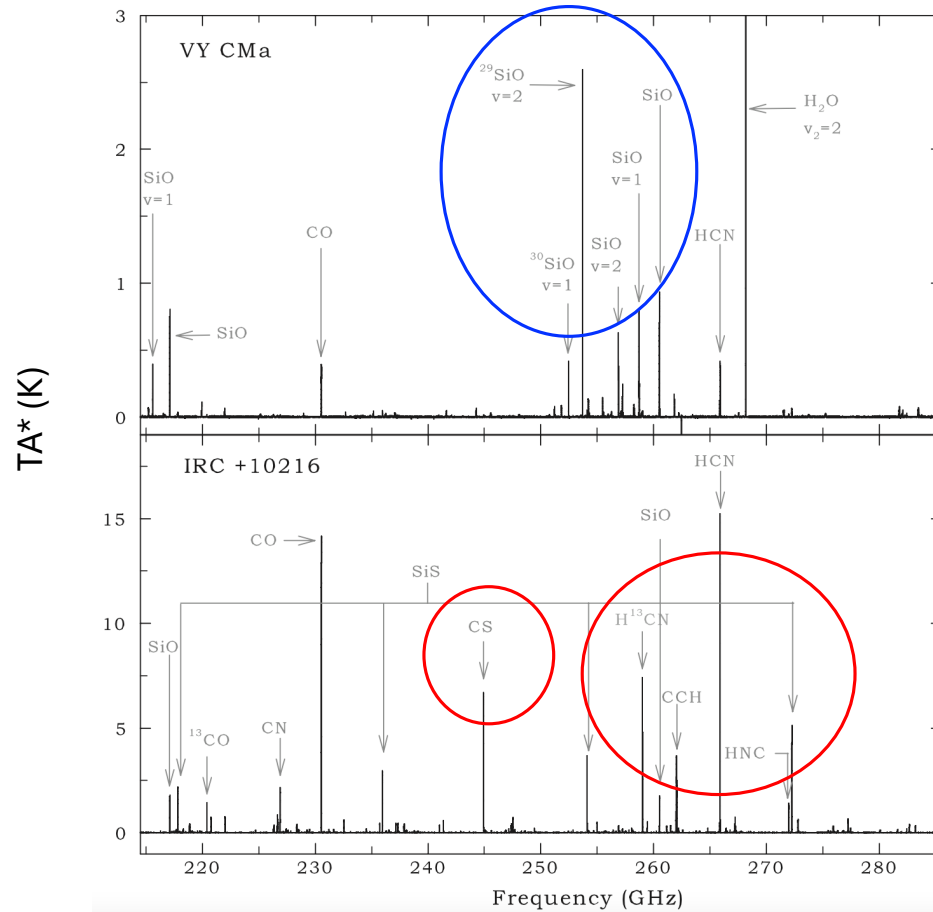
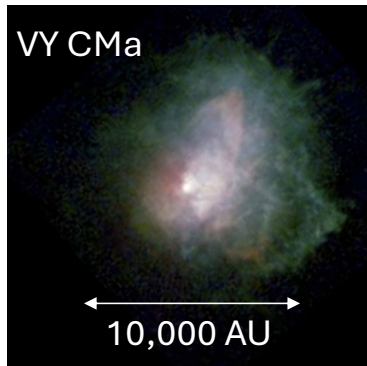


Rich in large carbon-chain and silicon-rich molecules!

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C-rich vs. O-rich



O-rich: H_2O , SiO , CO

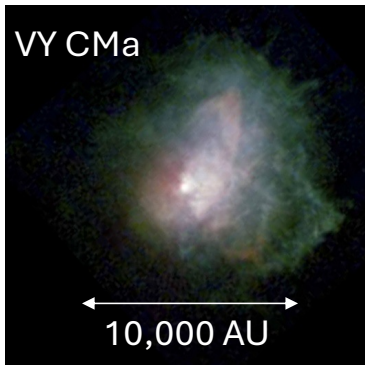
C-rich: CO , HCN ,
 H_2C_2 , SiS , CS , CH_4

Tenenbaum et al., 2010

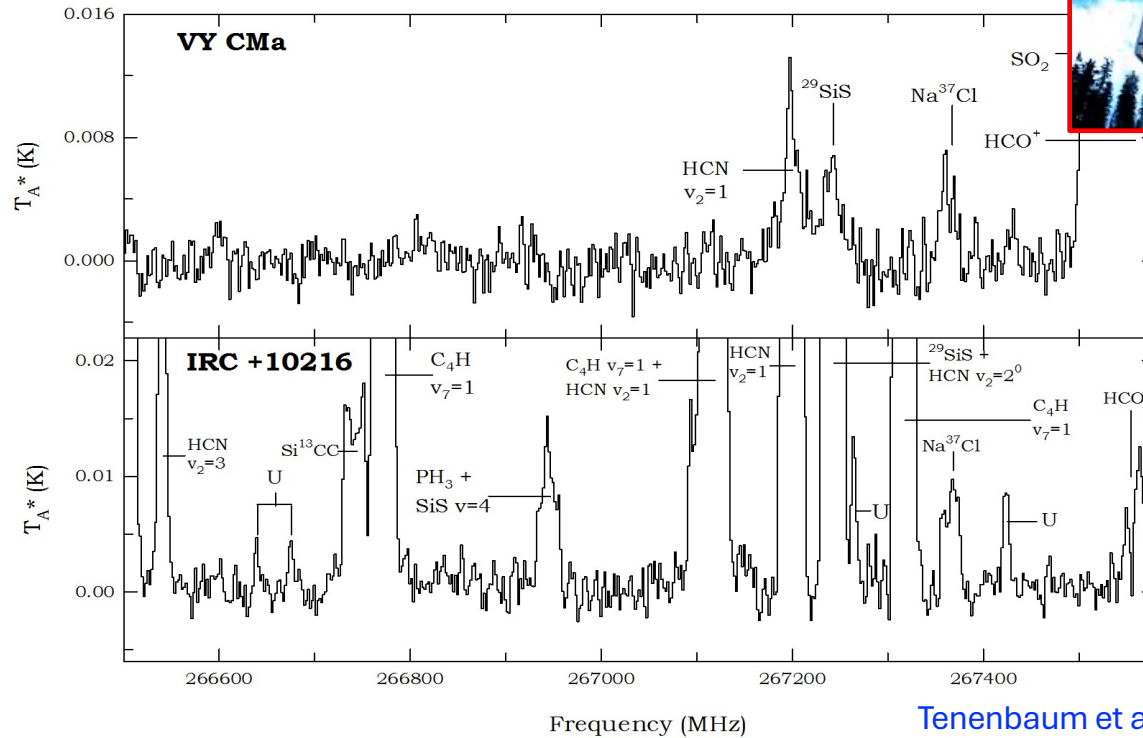
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C-rich vs. O-rich



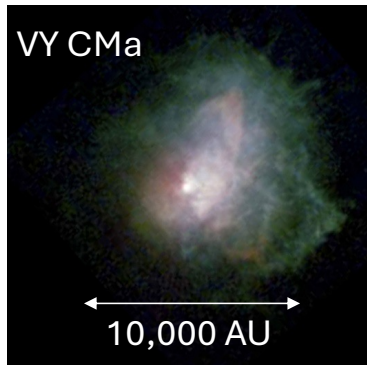
- VY CMa Spectrum dominated by **SO₂, SiO, SiS**
- IRC+10216 Spectrum dominated by **C₄H, HCN**



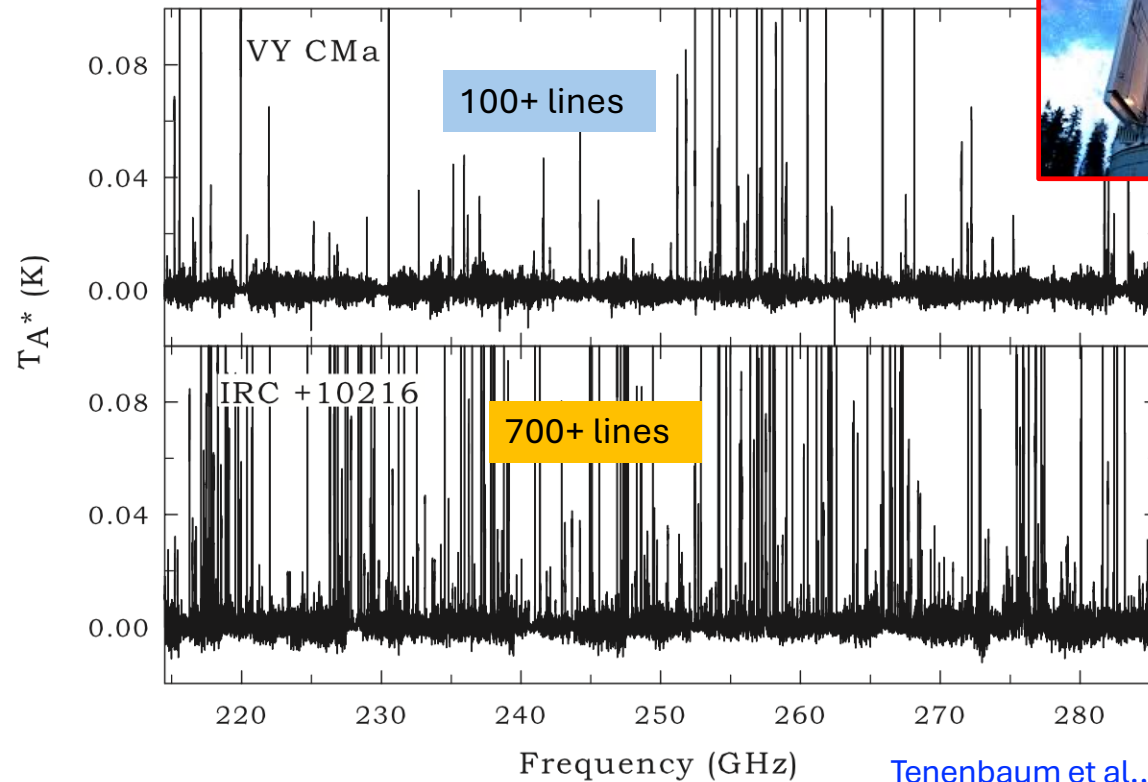
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C-rich vs. O-rich



Both objects overall **very** line rich!



*NOTE: VY Cma is ~10x farther away!!!

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Molecular Line Data

Planetary Nebula

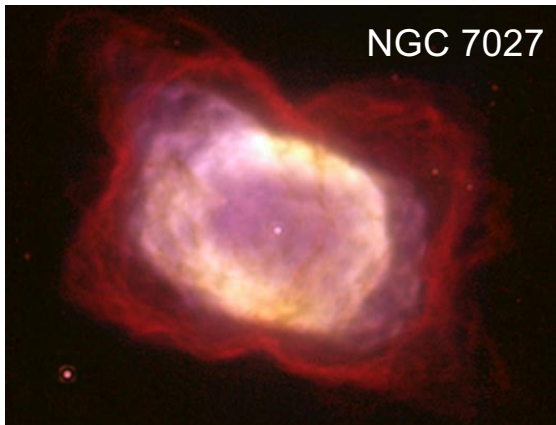


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Molecular Line Data

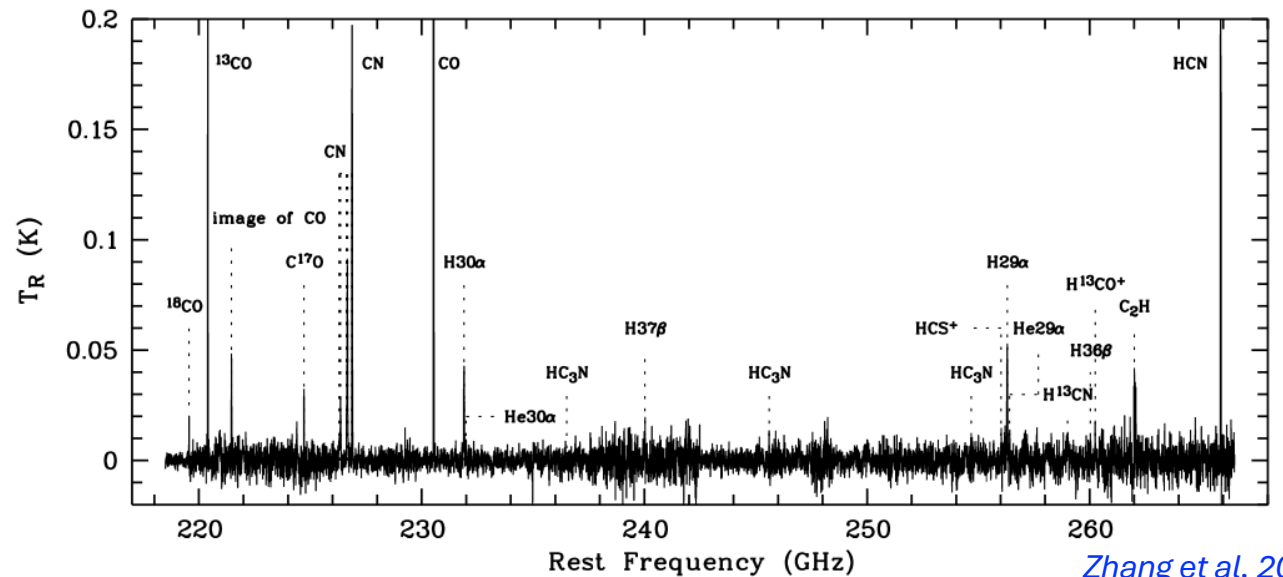
Planetary Nebula



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

Molecular Content:

CO, CN, HCN, HCO⁺, N₂H⁺, CCH, C₃H₂, HC₃N, OH, CH, CH⁺



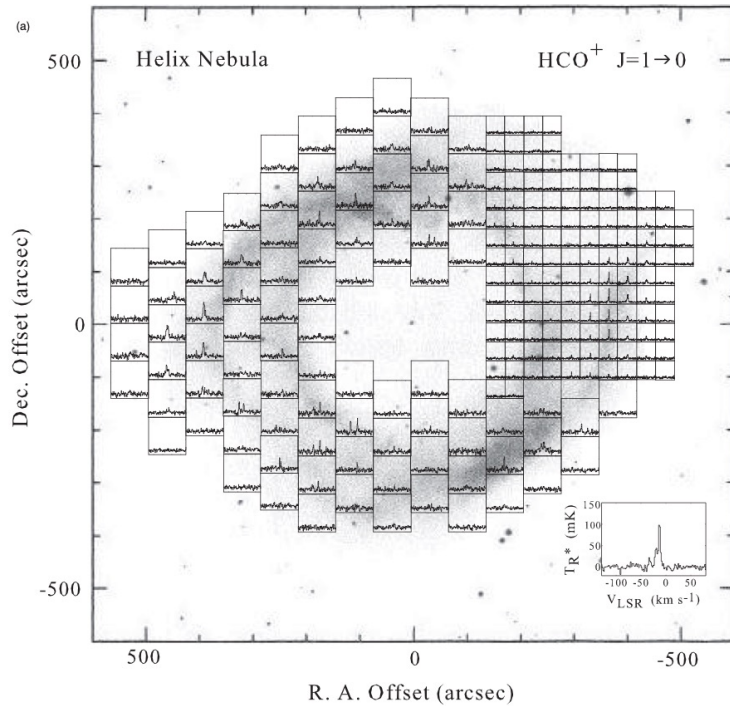
Zhang et al. 2008

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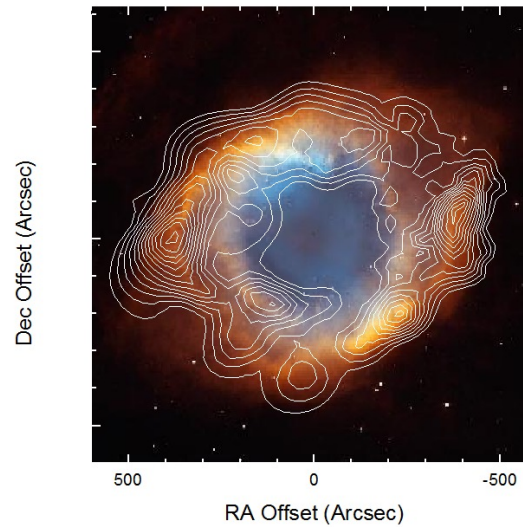


Molecular Line Data

Oldest Known Planetary Nebula: **The Helix**



Planetary Nebula



Zeigler et al., 2013

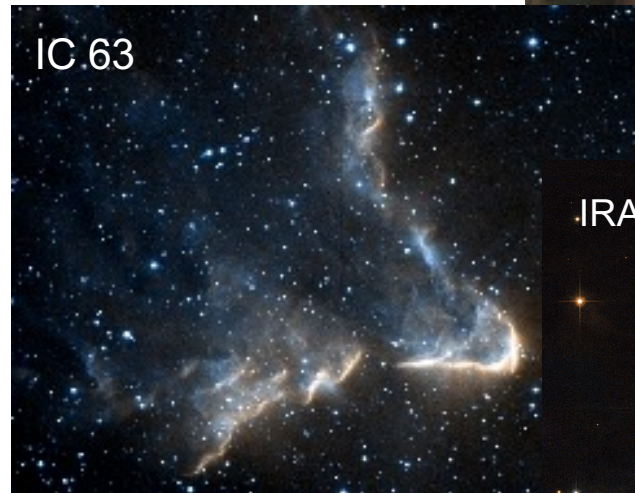
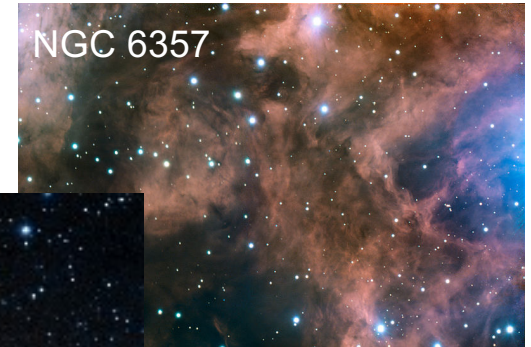
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Lack a *Definite Morphology*

- 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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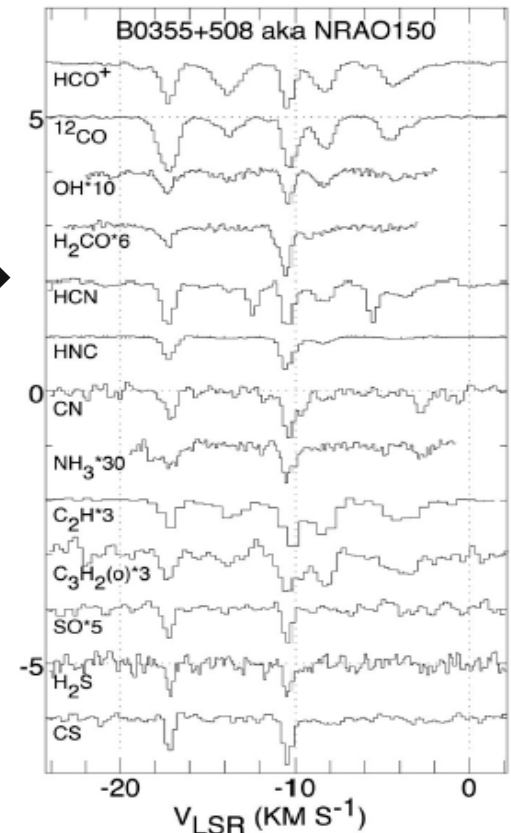
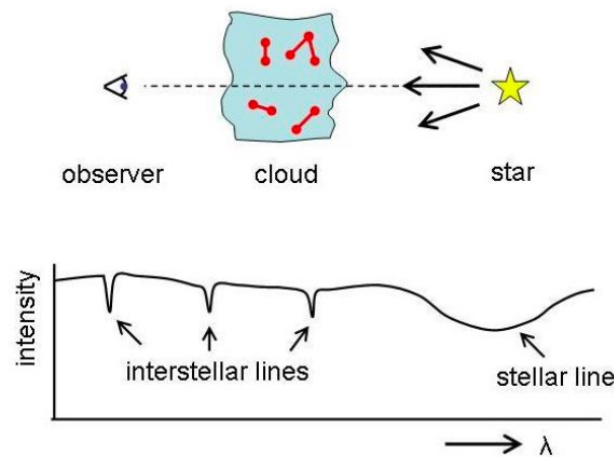
Diffuse Clouds

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
- Densities low: No radio/mm emission lines
- Not sufficient density for collisional excitation
- Molecules observed in ABSORPTION
- Common molecules observed

OH, H₂ (HD), CH, C₂, CH⁺, NH,
CO, H₃⁺

*line of sight to the blazar/radio-continuum source →



Credit: L. Ziurys

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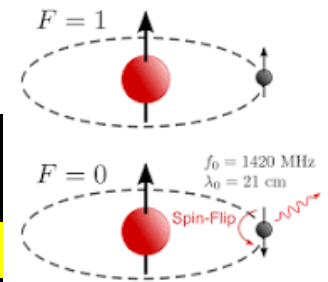
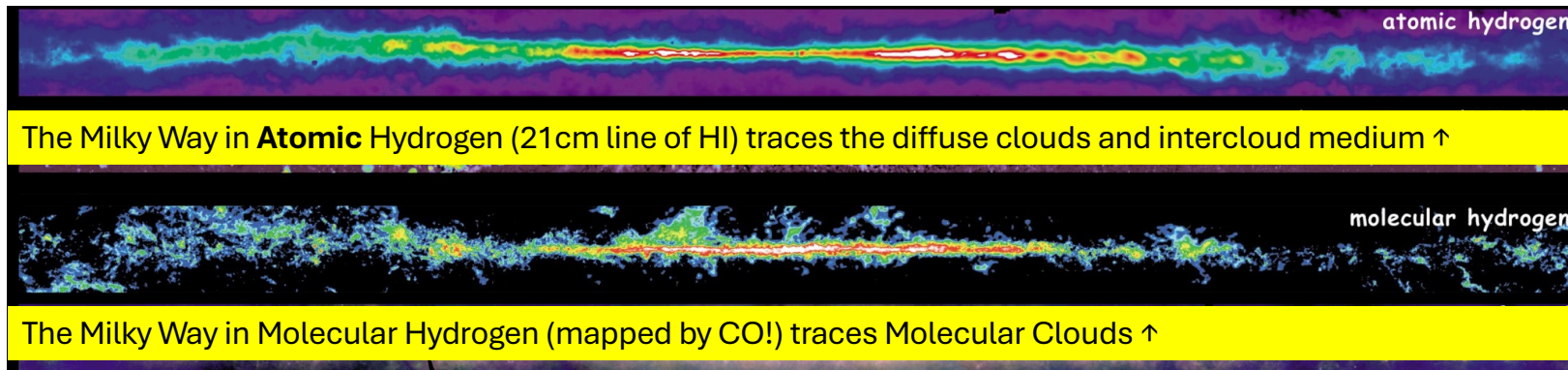


Lack a *Definite Morphology*

- 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

Diffuse Clouds

- Best traced by **21 cm HI line**
- $T_k \sim 100 \text{ K}$
- $n \sim 1 - 100 \text{ particles/cm}^3$ ($\text{H}^0 + \text{H}_2$)
- $x_e \sim 10^{-3}$ (*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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