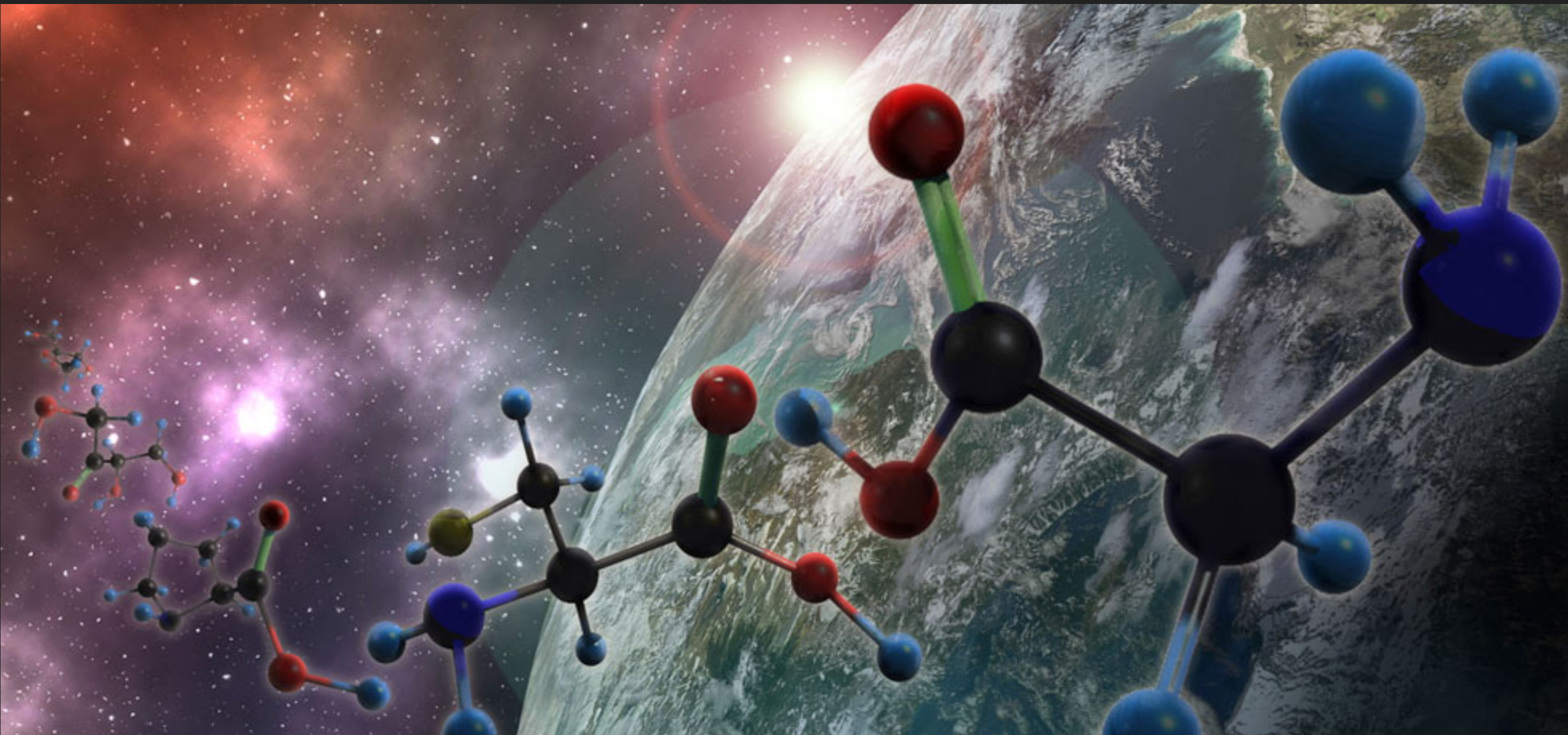


# LECTURE 1

STEFANO BOVINO,

UNIVERSIDAD DE CONCEPCIÓN



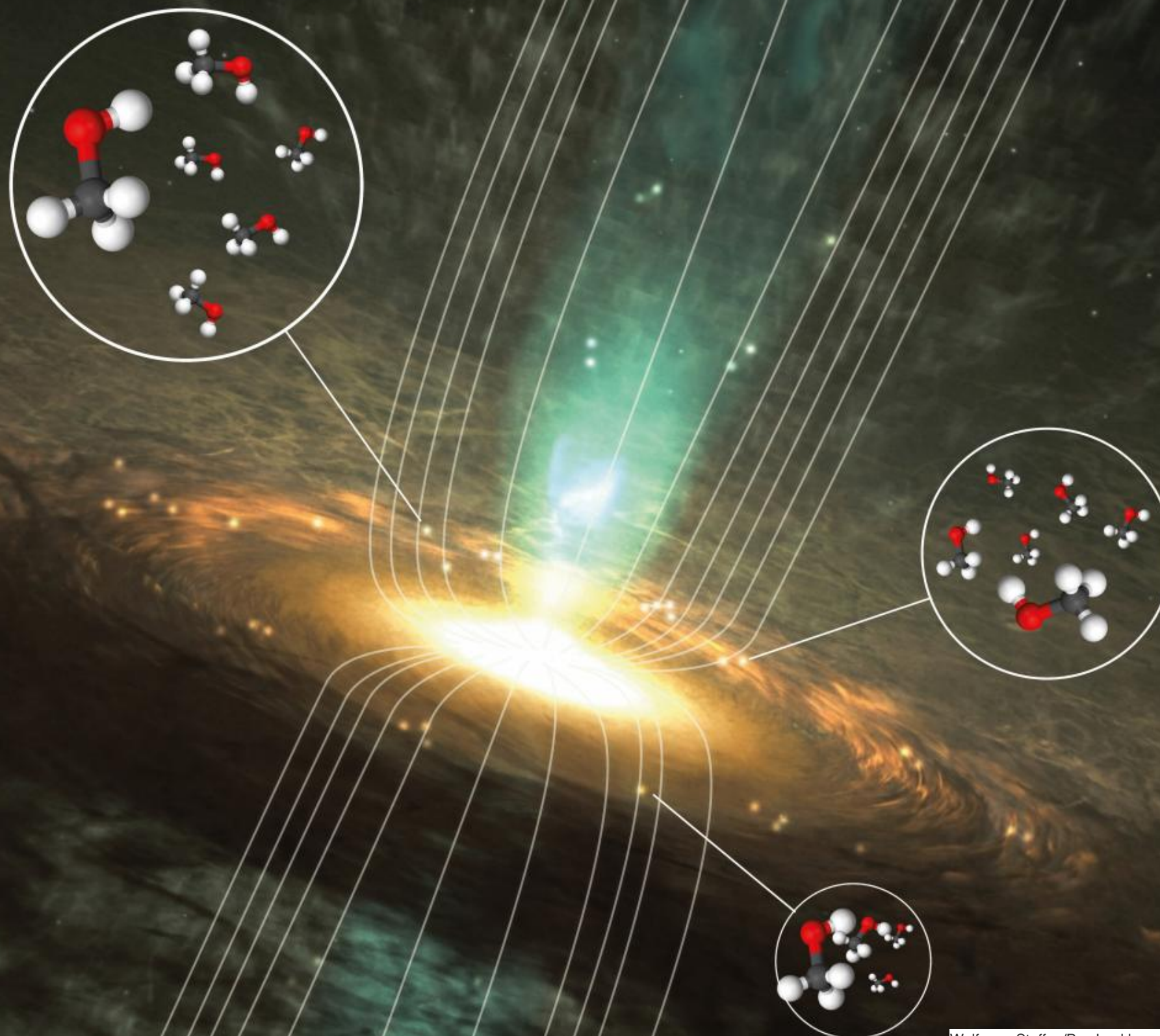
## FILL IT PLEASE





# WHAT IS ASTROCHEMISTRY?

3



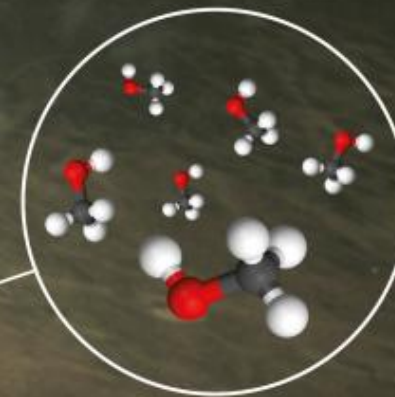
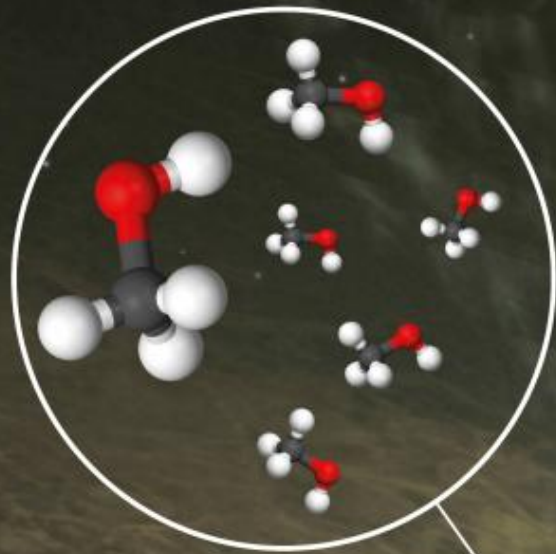
THE STUDY OF HOW MOLECULES AND  
CHEMICAL PROCESSES AFFECT THE DYNAMICS  
OF GALAXIES, STARS AND PLANETS  
FORMATION!



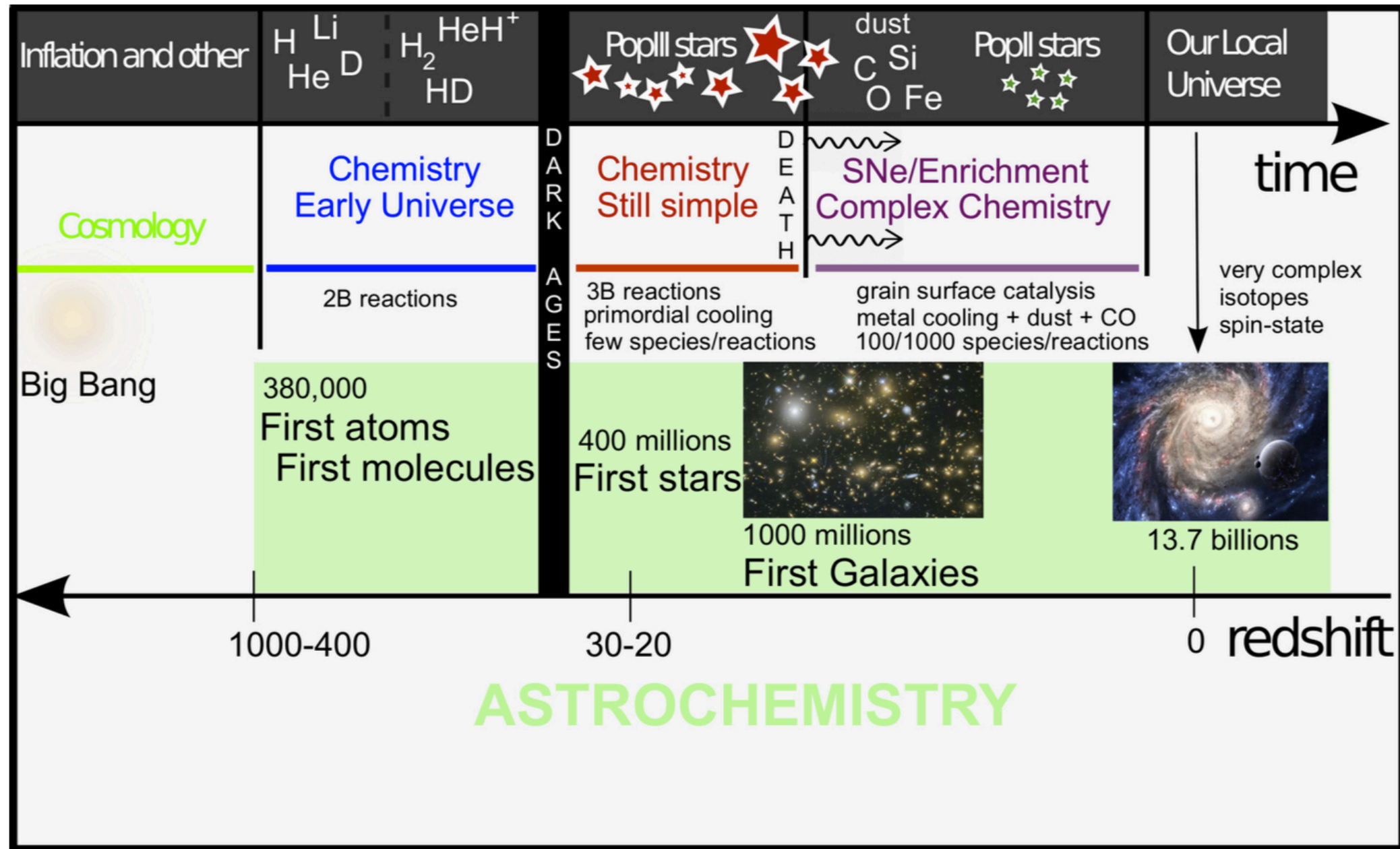


# WHEN DID ASTROCHEMISTRY START? <sup>5</sup>

## A BIT OF HISTORY



IT DOES EXIST SINCE EVER (~13.7 BILLIONS YEARS - SOMETHING)





# THE MOLECULAR UNIVERSE TIMELINE

Optical absorption lines of interstellar clouds towards bright stars!

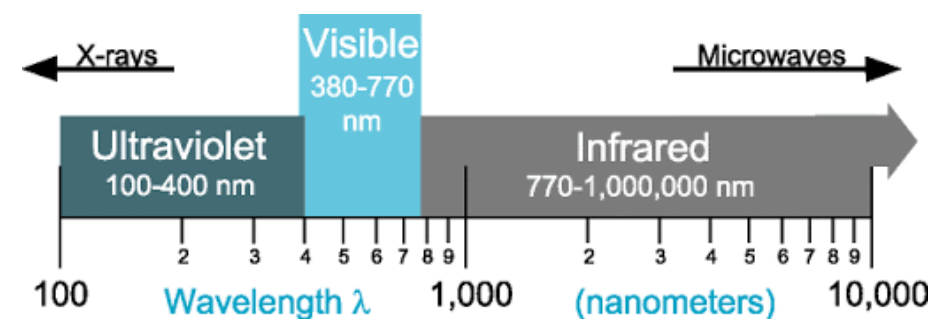
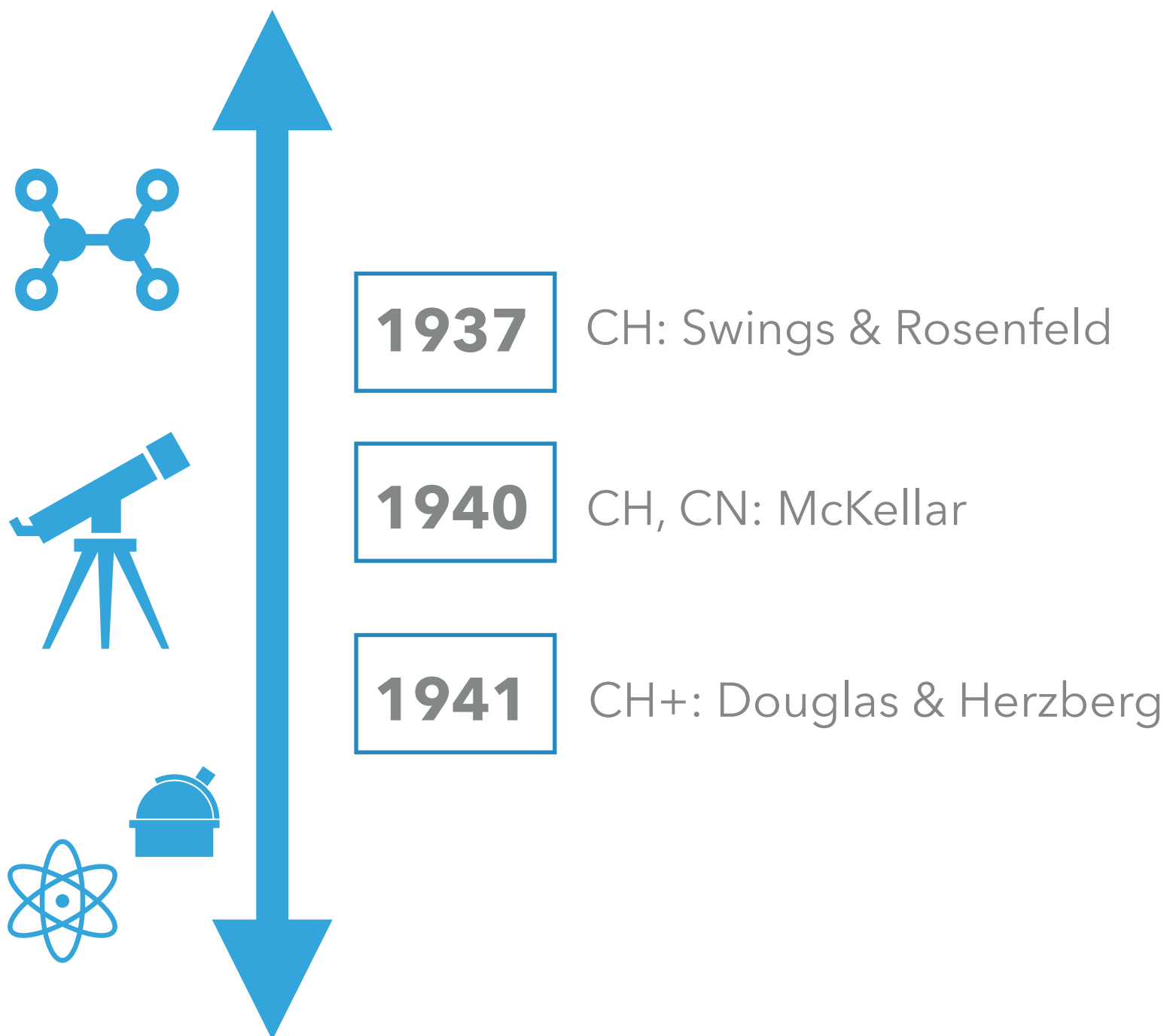


Fig. 1.1 The optical portion of the electromagnetic spectrum

**Spectral lines in optical band (300 GHz and 3000 THz)**

## THE MOLECULAR UNIVERSE TIMELINE

**1937-1939**

Eddington and Stromgren suggested the existence of H<sub>2</sub>

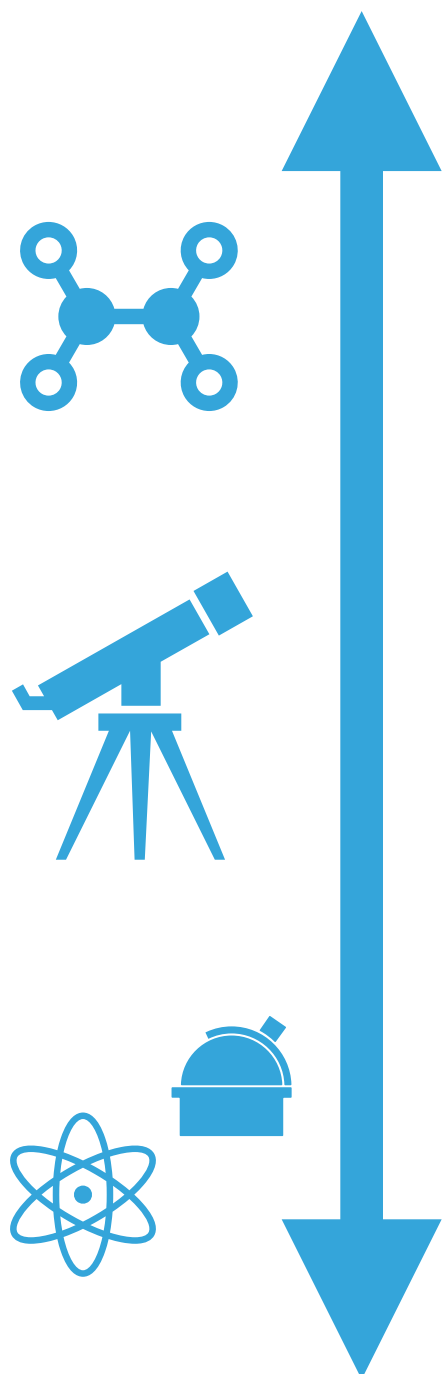
*I write about molecules with great diffidence, having not yet rid myself of the tradition that atoms are physics, but molecules are chemistry, but the new conclusion that hydrogen is abundant seems to make it likely that the above mentioned elements H, O, and N will frequently form molecules.*

Sir A.S. Eddington 1937

Thirty years later, Gould & Salpeter (1963) and Hollenbach et al. (1971) predicted that it could be a large fraction of all hydrogen (studying formation of H<sub>2</sub> on the surface of grains.



# THE MOLECULAR UNIVERSE TIMELINE



**1946-1951**

First astrochemical models (Kramers, Bates & Spitzer)

BULLETIN OF THE ASTRONOMICAL INSTITUTES  
OF THE NETHERLANDS

1946 April 30

Volume X

No. 371

COMMUNICATION FROM THE OBSERVATORY AT LEIDEN

Condensation in interstellar space, by *H. A. Kramers* and *D. ter Haar* <sup>1)</sup>.

# THE MOLECULAR UNIVERSE TIMELINE

BULLETIN OF THE ASTRONOMICAL SOCIETY

INSTITUTES

## THE ASTROPHYSICAL JOURNAL

AN INTERNATIONAL REVIEW OF SPECTROSCOPY AND  
ASTRONOMICAL PHYSICS

1946 April

COI

NUMBER 3 No. 371

EIDEN

Conder.

MAY 1951

(*adv* 1).

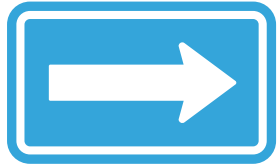
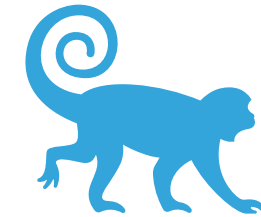
VOLUME 113

THE DENSITY OF MOLECULES IN INTERSTELLAR SPACE  
DAVID R. BATES\* AND LYMAN SPITZER, JR.  
University College, London, and Princeton University Observatory  
Received January 22, 1951



# THE MOLECULAR UNIVERSE TIMELINE

Primate Astrochemistry



1946-1951

First astrochemical models (Kramers, Bates & Spitzer)

FIGURE I

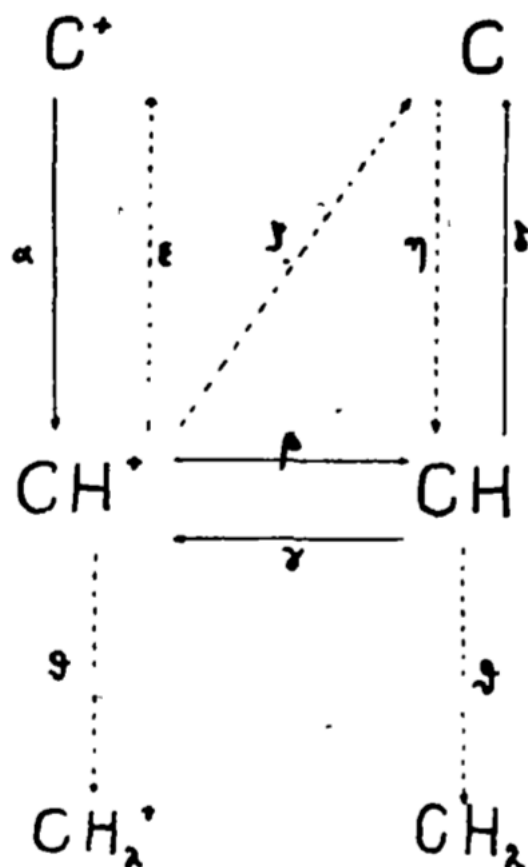
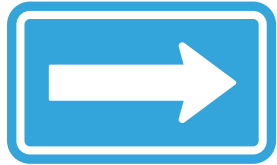


TABLE I

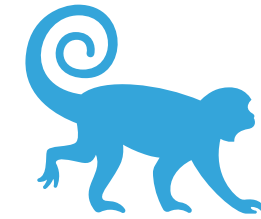
Process	Description	Frequency
$\alpha : C^+ + H \rightarrow CH^+ + h\nu$	(radiation capture)	$N_\alpha = 10^{-17} \cdot \rho_{C^+} \cdot \rho_H$
$\beta : CH^+ + e \rightarrow CH + h\nu$	(electron capture)	$N_\beta = 3 \cdot 10^{-13} \cdot \rho_{e^-} \cdot \rho_{CH^+}$
$\gamma : CH + h\nu \rightarrow CH^+ + e$	(photoionization)	$N_\gamma = 2 \cdot 10^{-11} \cdot \rho_{CH}$
$\delta : CH + h\nu \rightarrow C + H$	(photodissociation)	$N_\delta = 10^{-11} \cdot \rho_{CH}$
$\epsilon : CH^+ + h\nu \rightarrow C^+ + H$	(photodissociation)	$N_\epsilon \sim 10^{-15} \cdot \rho_{CH^+}$
$\zeta : CH^+ + e \rightarrow C + H$	(electron capture leading to dissociation)	$N_\zeta \sim 3 \cdot 10^{-14} \cdot \rho_{e^-} \cdot \rho_{CH^+}$
$\eta : C + H \rightarrow CH + h\nu$	(radiation capture)	$N_\eta = 7 \cdot 10^{-18} \cdot \rho_C \cdot \rho_H$
$\zeta' : CH^{(+)} + H \rightarrow CH_2^{(+)}$	("mechanical" capture)	$N_{\zeta'} \leq 7 \cdot 10^{-17} \cdot \rho_{CH^{(+)}} \cdot \rho_H$

# WHEN THE FIRST ASTROCHEMICAL MODELS?



**1946-1951**

First astrochemical models (Kramers, Bates & Spitzer)



**Primate Astrochemistry**

TABLE 2

PROCESS	RATE COEFFICIENT	
	Designation	Value
a) $C + H \rightarrow CH + h\nu \dots\dots\dots$	$\gamma_1$	$\begin{cases} 2 \times 10^{-18} \text{ cm}^3/\text{sec} [\frac{1}{9}C(^3P_0 + 3^3P_1 + 5^3P_2)] \\ 6 \times 10^{-18} \text{ cm}^3/\text{sec} [C(^3P_0)] \end{cases}$
b) $C^+ + H \rightarrow CH^+ + h\nu \dots\dots\dots$	$\gamma_2$	$\begin{cases} 2 \times 10^{-18} \text{ cm}^3/\text{sec} [\frac{1}{3}C^+(^2P_{1/2} + 2^2P_{3/2})] \\ 0 [C^+(^2P_{1/2})] \end{cases}$
c) $CH + h\nu \rightarrow CH^+ + e \dots\dots\dots$	$\beta_1$	$8 \times 10^{-12} \text{ sec}^{-1}$
d) $CH^+ + e \rightarrow CH + h\nu$	$a_1$	$7 \times 10^{-12} \text{ cm}^3/\text{sec}$
e) $CH^+ + e \rightarrow CH' + h\nu$		
$CH' \rightarrow \begin{cases} \text{(i) } CH + h\nu \\ \text{(ii) } C + H \end{cases}$	$a_2$	Unknown (probably small but conceivably large)
f) $CH^+ + e \rightarrow C + H \dots\dots\dots$	$\beta_2$	$n(CH) = n(H) \left[ \frac{\gamma_1 \{ (a_1 + a_2) n(e) + \beta_3 \} n(C) + \gamma_2 a_1 n(e) n(C^+)}{\beta_3 (\beta_1 + \beta_2) + \{ \beta_1 a_2 + \beta_2 (a_1 + a_2) \} n(e)} \right]$
g) $CH + h\nu \rightarrow C + H \dots\dots\dots$	$\beta_3$	
h) $CH + h\nu \rightarrow C^+ + H \dots\dots\dots$		

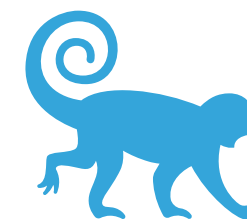
$$n(CH^+) = n(H) \left[ \frac{\gamma_1 \beta_1 n(C) + \gamma_2 (\beta_1 + \beta_2) n(C^+)}{\beta_3 (\beta_1 + \beta_2) + \{ \beta_1 a_2 + \beta_2 (a_1 + a_2) \} n(e)} \right],$$

## WHEN THE FIRST ASTROCHEMICAL MODELS?



**1946-1951**

First astrochemical models (Kramers, Bates & Spitzer)



**Primate Astrochemistry**

1. From these models it was already clear that detection contained important astrophysical information
2. These studies provided useful probes of interstellar regions
3. For instance: CH and CN were easily explained by equilibrium models while CH<sup>+</sup> required more dynamics (e.g. post-shock chemistry)
4. Two types of interstellar regions:

$t_{\text{chem}} < t_{\text{dyn}}$  (equilibrium) and  $t_{\text{chem}} > t_{\text{dyn}}$  (non-eq) [VERY IMPORTANT]

## THE MOLECULAR UNIVERSE TIMELINE (RADIO AND UV ASTRONOMY)

For various reasons (distraction towards space flight)  
no real development during 1941-1969

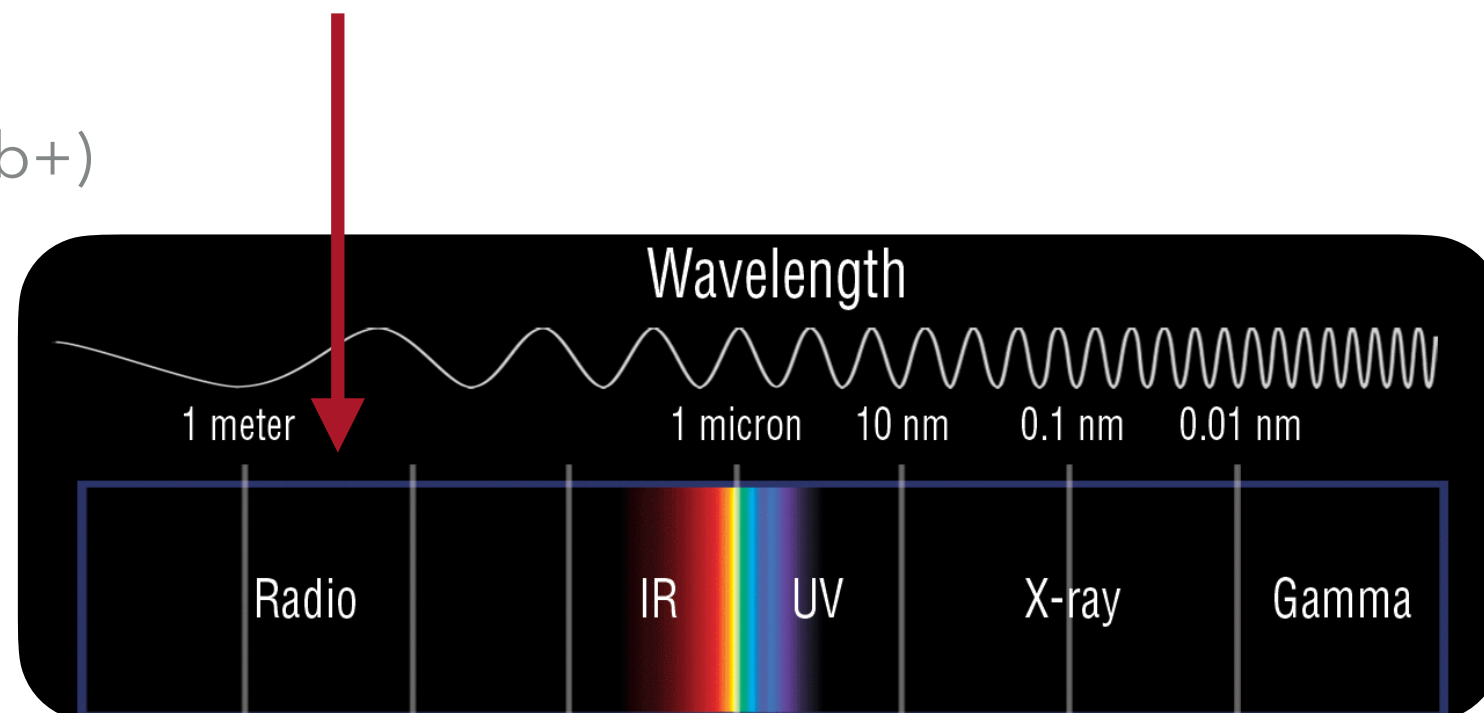
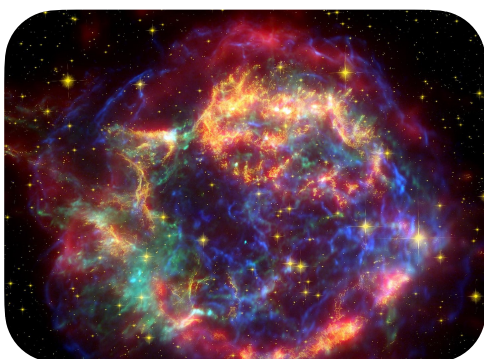
**Late '60**

Development of radioastronomy which started during WWII  
**Rotational spectroscopy**

**1963**

OH (in radio at 18 cm by Weinreb+)

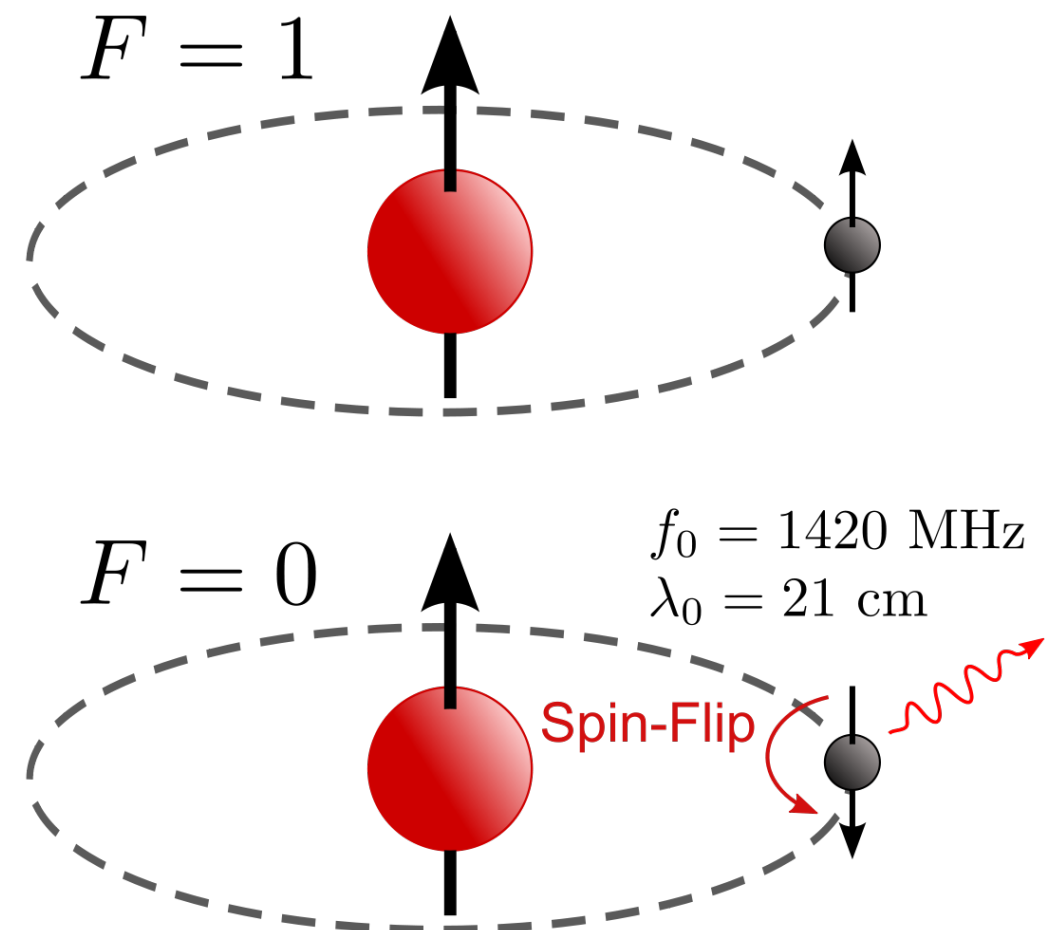
towards SNR Cassiopeia A



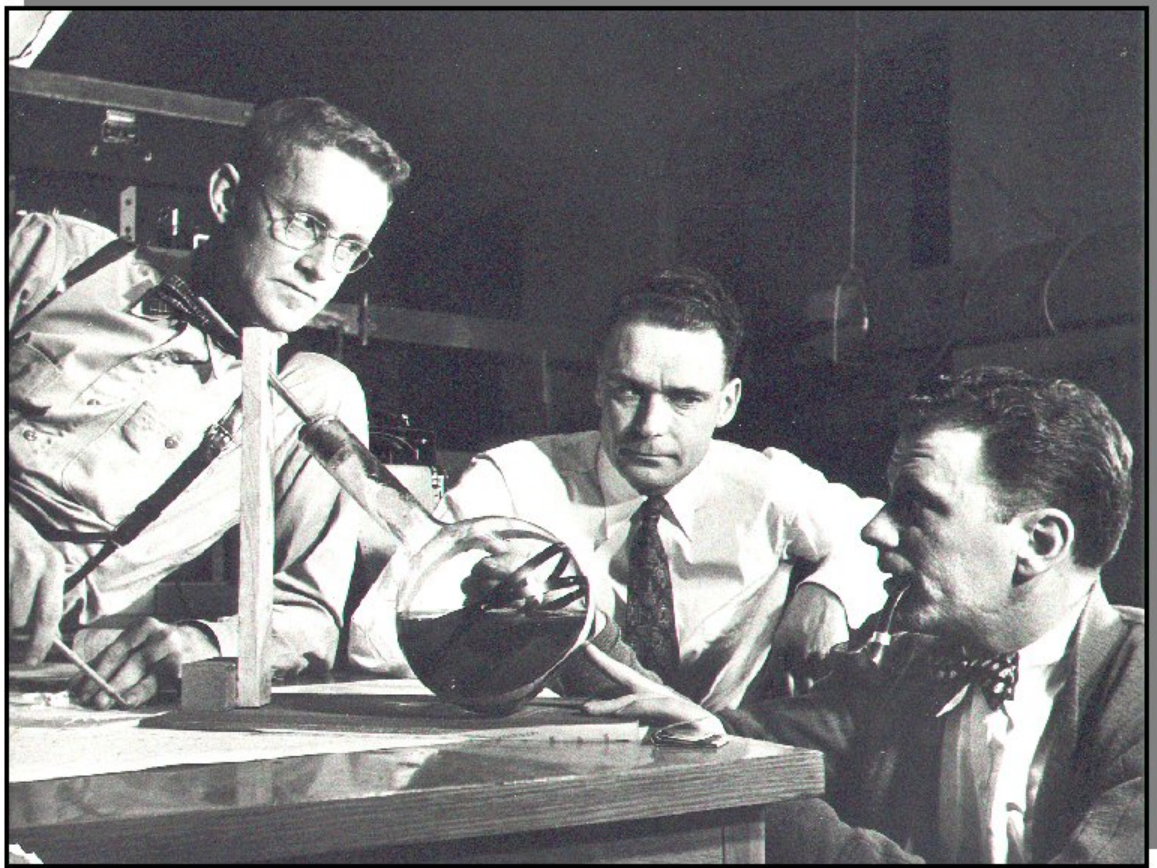


# Radioastronomy & HI 21 cm line

**1944** - Hendrik van de Hulst predicts the existence of the HI 21-cm



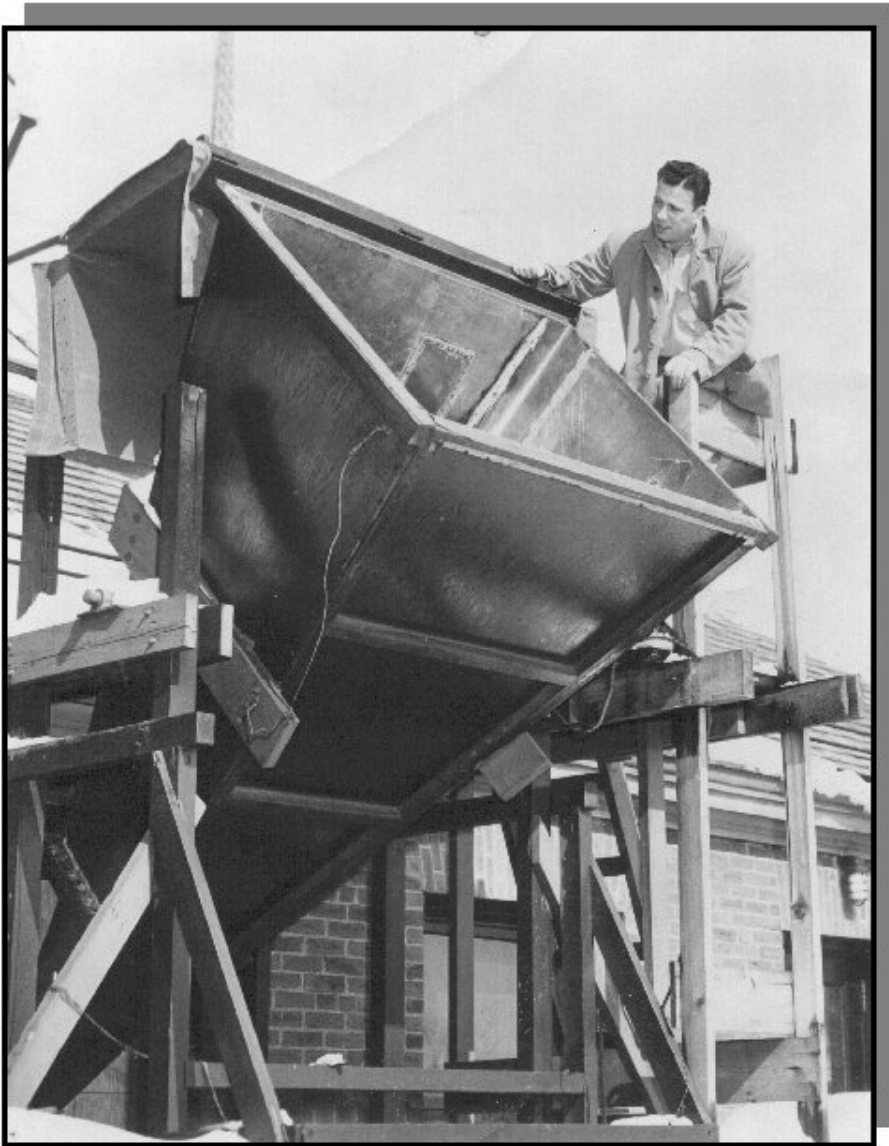
1950 - Doc Ewen worked 40 hours a week to design and build the apparatus for the new cyclotron at Harvard



- + he has to complete his PhD (working at nights and week-ends)
- + Building a receiver to detect 21 cm HI line (supervised by Purcell)



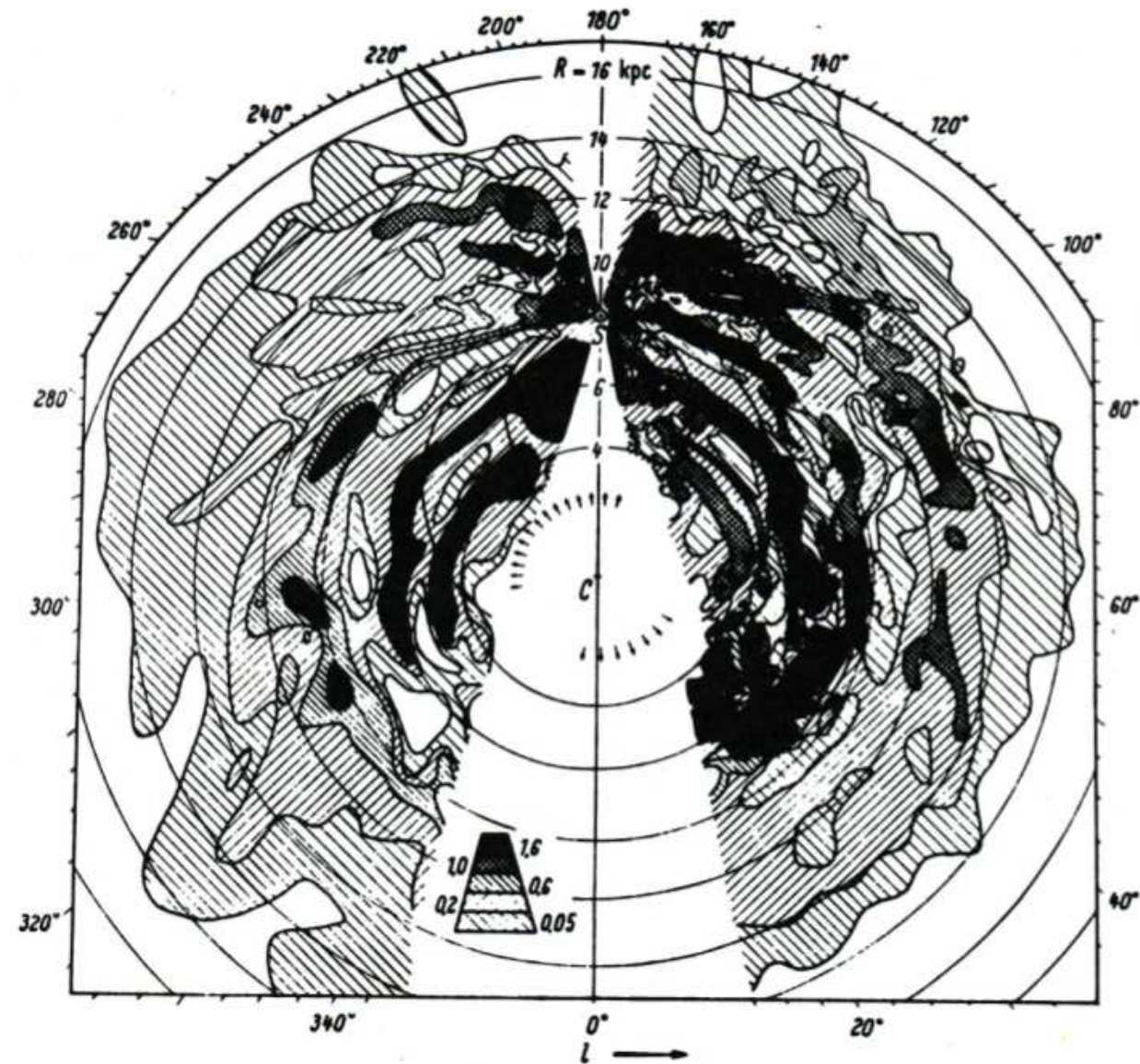
## 1950-1951- Purcell received 500 USD to build the antenna



6 weeks later - Muller & Oort confirmed the detection

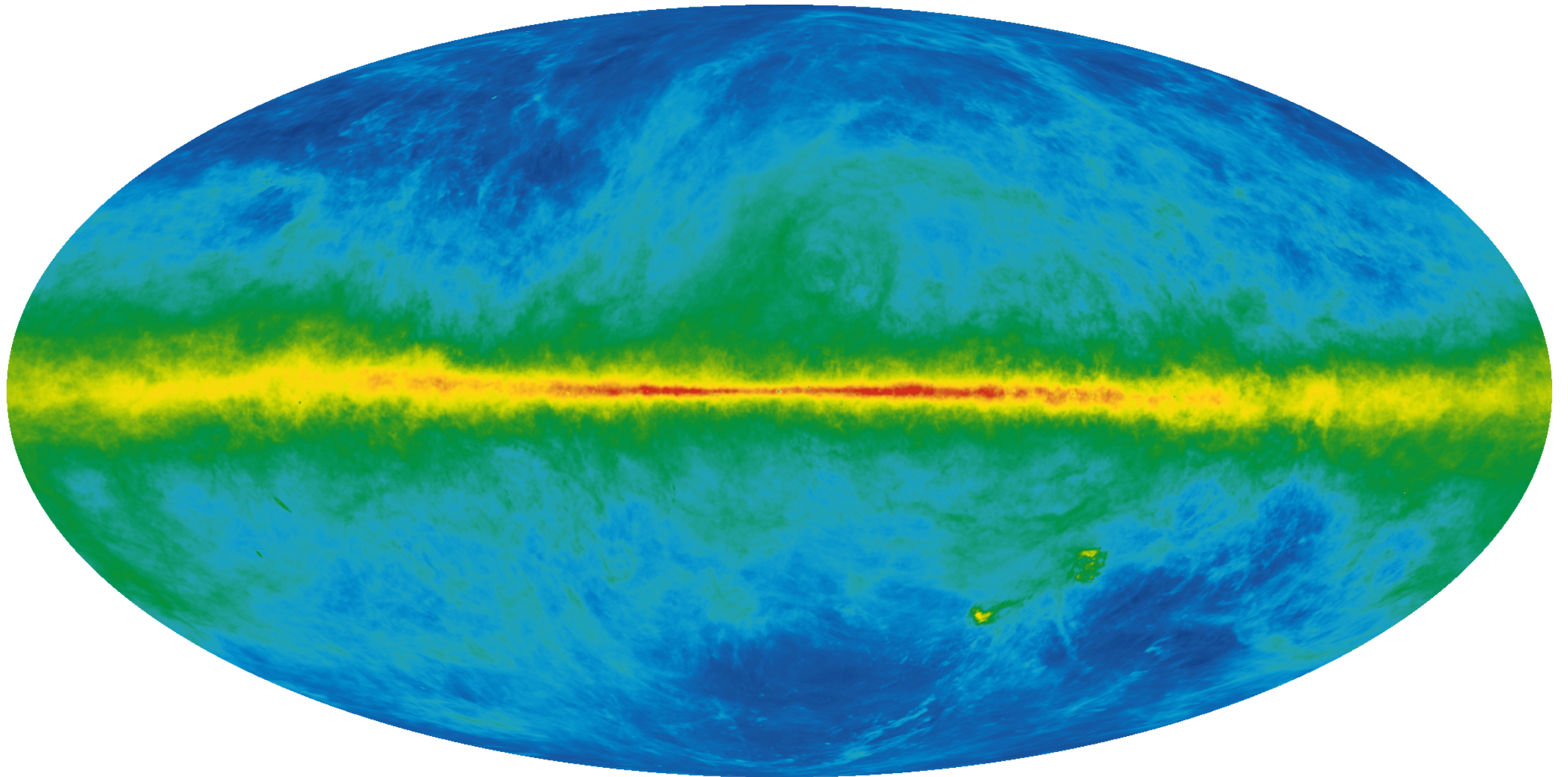


# Discovery of spiral arms (neutral HI)



Oort, 1958

Cold HI emitting @ 21-cm makes up most of the mass of the ISM gas in the Milky Way  
Its observation represented a revolution





## THE MOLECULAR UNIVERSE TIMELINE (RADIO AND UV ASTRONOMY)

**1968**

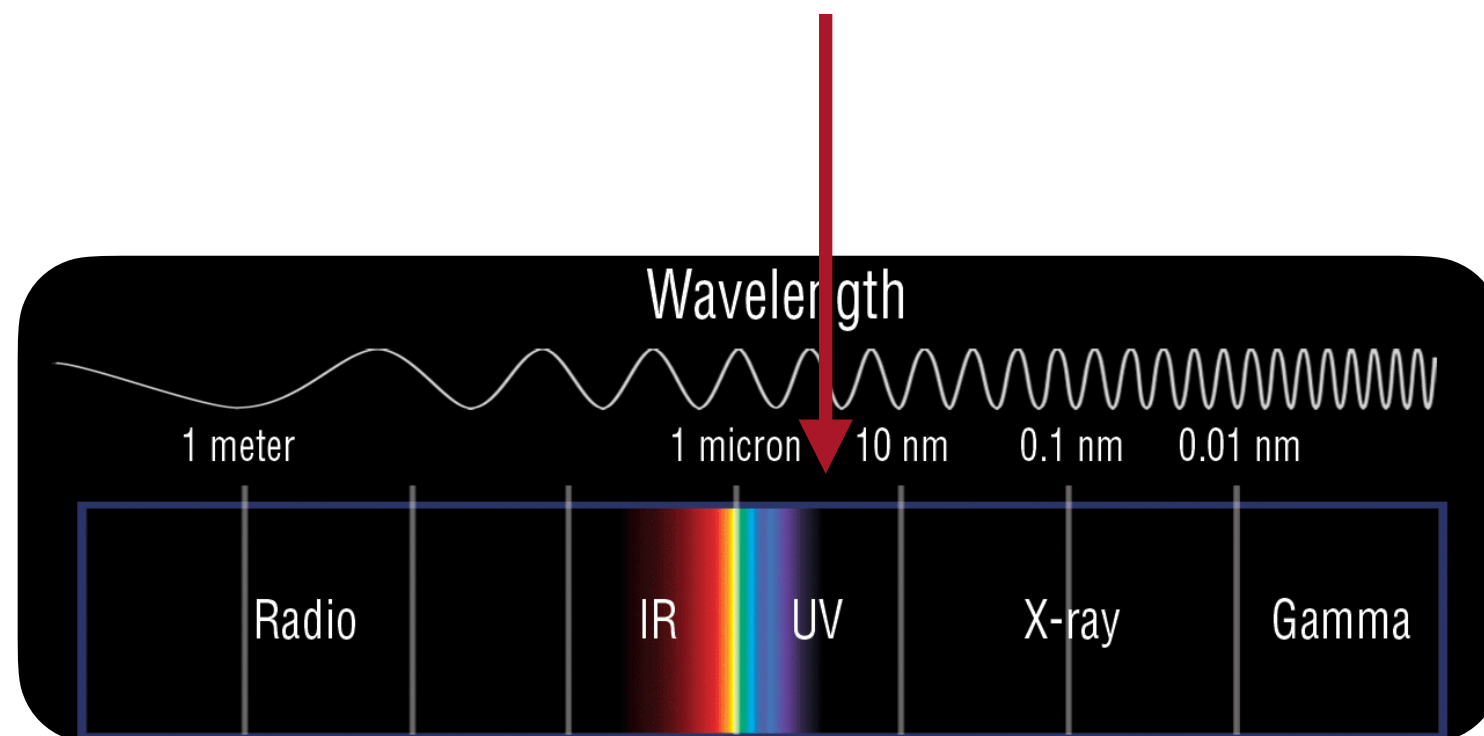
NH<sub>3</sub> (First polyatomic molecule in radio @ 1 cm by Cheung, Townes+)

**1969**

H<sub>2</sub>O (Cheung+ at 1 cm, i.e. 22 GHz)

**>1970**

Development of UV astronomy + mm (first detection of H<sub>2</sub> and CO)





## THE MOLECULAR UNIVERSE TIMELINE (RADIO AND UV ASTRONOMY)

1970

H<sub>2</sub> (Carruthers, First detection in absorption towards the star zeta-Persei,  $N[\text{H}_2] \sim 1.3 \times 10^{20} \text{ cm}^{-2}$ )

1973

H<sub>2</sub> (Smith in absorption towards delta-Scorpii  $N[\text{H}_2] \sim 3 \times 10^{19} \text{ cm}^{-2}$ )

### ROCKET OBSERVATION OF INTERSTELLAR MOLECULAR HYDROGEN

GEORGE R. CARRUTHERS

E. O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, D.C. 20390

*Received 1970 June 22*

#### ABSTRACT

The Lyman resonance-absorption bands of interstellar molecular hydrogen have been observed in the far-ultraviolet spectrum of the star  $\xi$  Persei. The column density of H<sub>2</sub> is estimated to be about  $1.3 \times 10^{20} \text{ cm}^{-2}$ . The column density of interstellar atomic hydrogen, determined from the L $\alpha$  absorption line in the same spectrum, is about  $4.2 \times 10^{20} \text{ cm}^{-2}$ . Hence, in this line of sight, where visual total extinction by dust is about 1 mag, nearly half of the total hydrogen may be in molecular form. This is in agreement with theoretical predictions.

### INTERSTELLAR MOLECULAR HYDROGEN OBSERVED IN THE ULTRAVIOLET SPECTRUM OF DELTA SCORPII

ANDREW M. SMITH

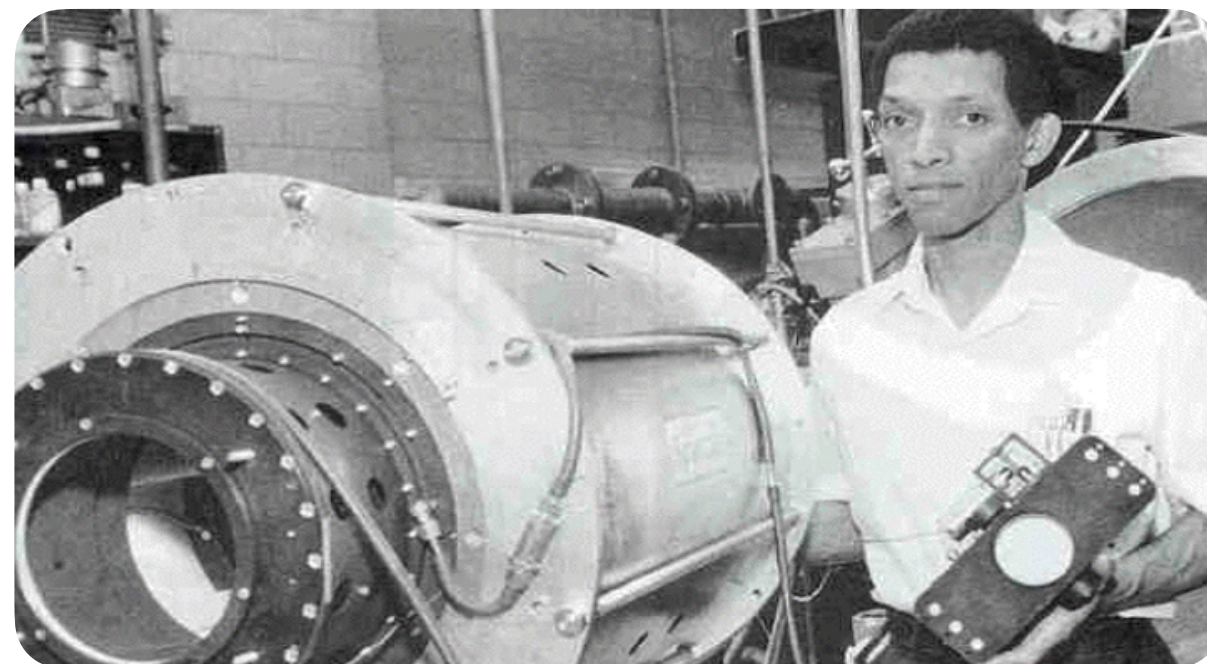
NASA, Goddard Space Flight Center,  
Greenbelt, Maryland

*Received 1972 October 26*

#### ABSTRACT

Molecular-hydrogen bands of the Lyman and Werner systems have been observed in the ultraviolet, interstellar spectrum of  $\delta$  Sco. The average molecular column density is  $3.5 (+2.2, -0.9) \times 10^{19} \text{ cm}^{-2}$ , and the average temperature of the gas of which the molecules are part is 47° K. Minimum and maximum gas temperatures are 25° and 98° K, respectively. The observed column density of hydrogen atoms is  $(1.5 \pm 0.5) \times 10^{21} \text{ cm}^{-2}$ , and hence the ratio of the number of hydrogen atoms in molecular form to the total number of hydrogen atoms in either atomic or molecular form is 0.044 (+0.070, -0.018).

*Subject headings:* interstellar medium — molecules, interstellar — ultraviolet — stars, individual



George Carruthers  
Pioneer of UV astronomy



> 1980

First mm surveys: discovery of many new molecules

# ORION MOLECULAR CLOUD (MM ASTRONOMY)

D = 400 pc

Nearby high-mass star-forming cloud with strong lines emission (HST image)

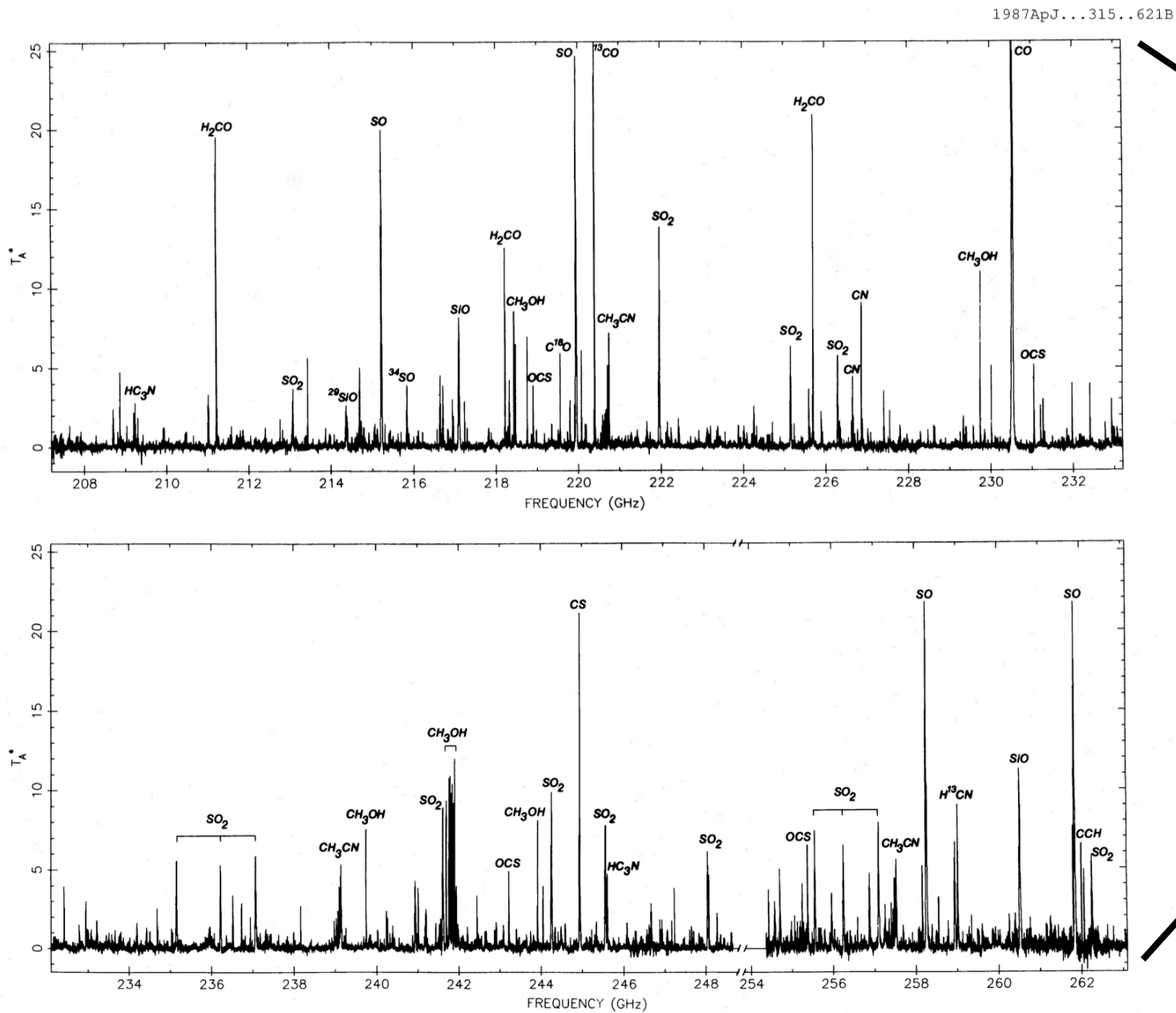


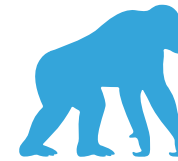
FIG. 1.—Compressed view of the OVRO spectral line survey of OMC-1



Sutton+1985, Blake+1986, Blake+1987



# THE MOLECULAR UNIVERSE TIMELINE (IR ASTRONOMY)



## Evolved Astrochemistry

**>1980**

Development of IR astronomy  
First full-sky survey @ 12, 25, 60, and 100 micron

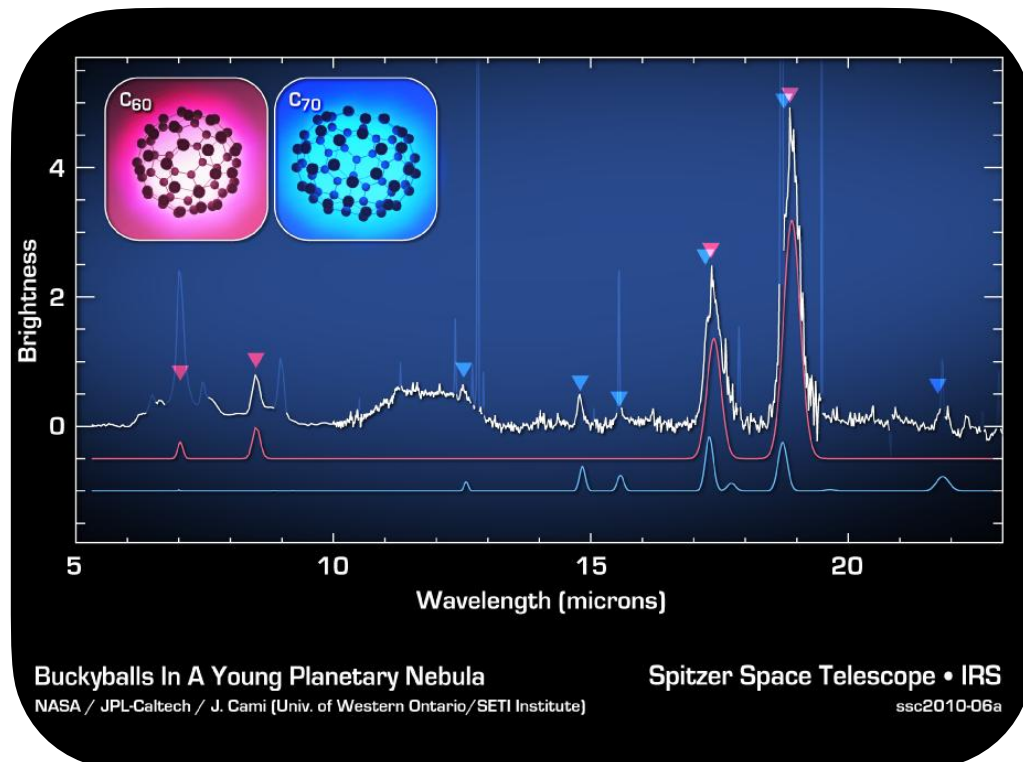
IRAS: obs. of dust particles and PAH

**1995-1998**

Infrared Space Obs. Nature and composition of grains, H<sub>2</sub> in shocks  
First survey at 2-200 micron (symm. mol. C<sub>6</sub>H<sub>6</sub>, CH<sub>3</sub>, C<sub>2</sub>H<sub>4</sub>, CO<sub>2</sub>)

**2003-2009**

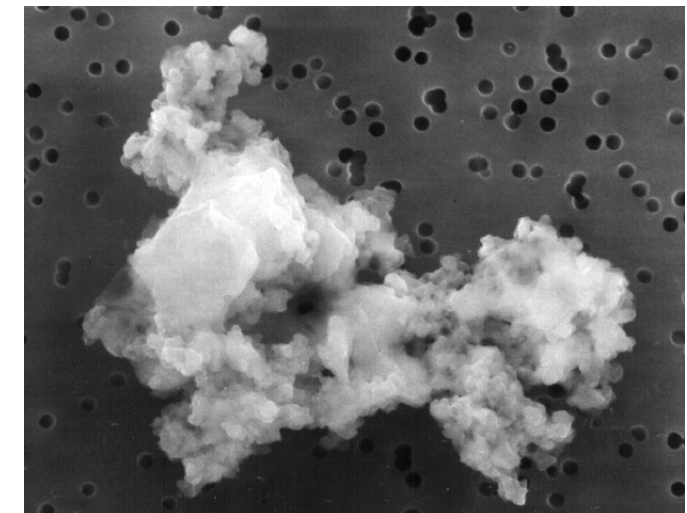
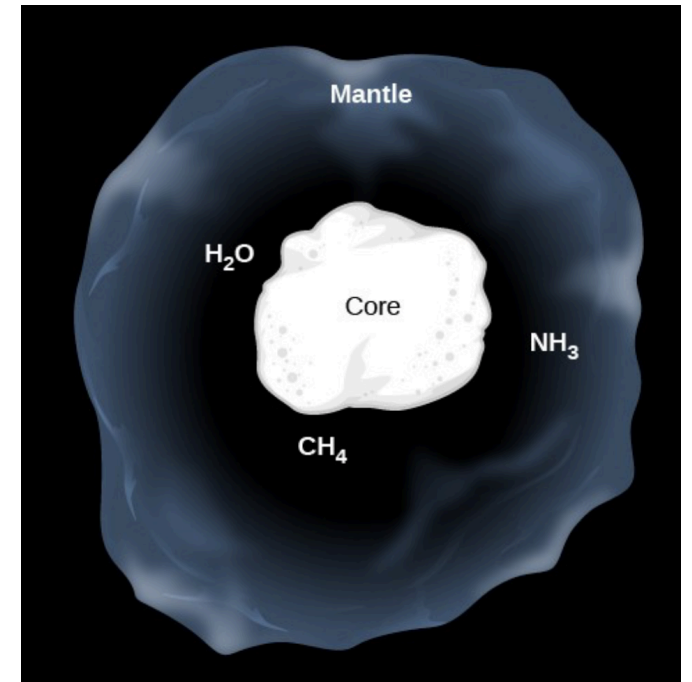
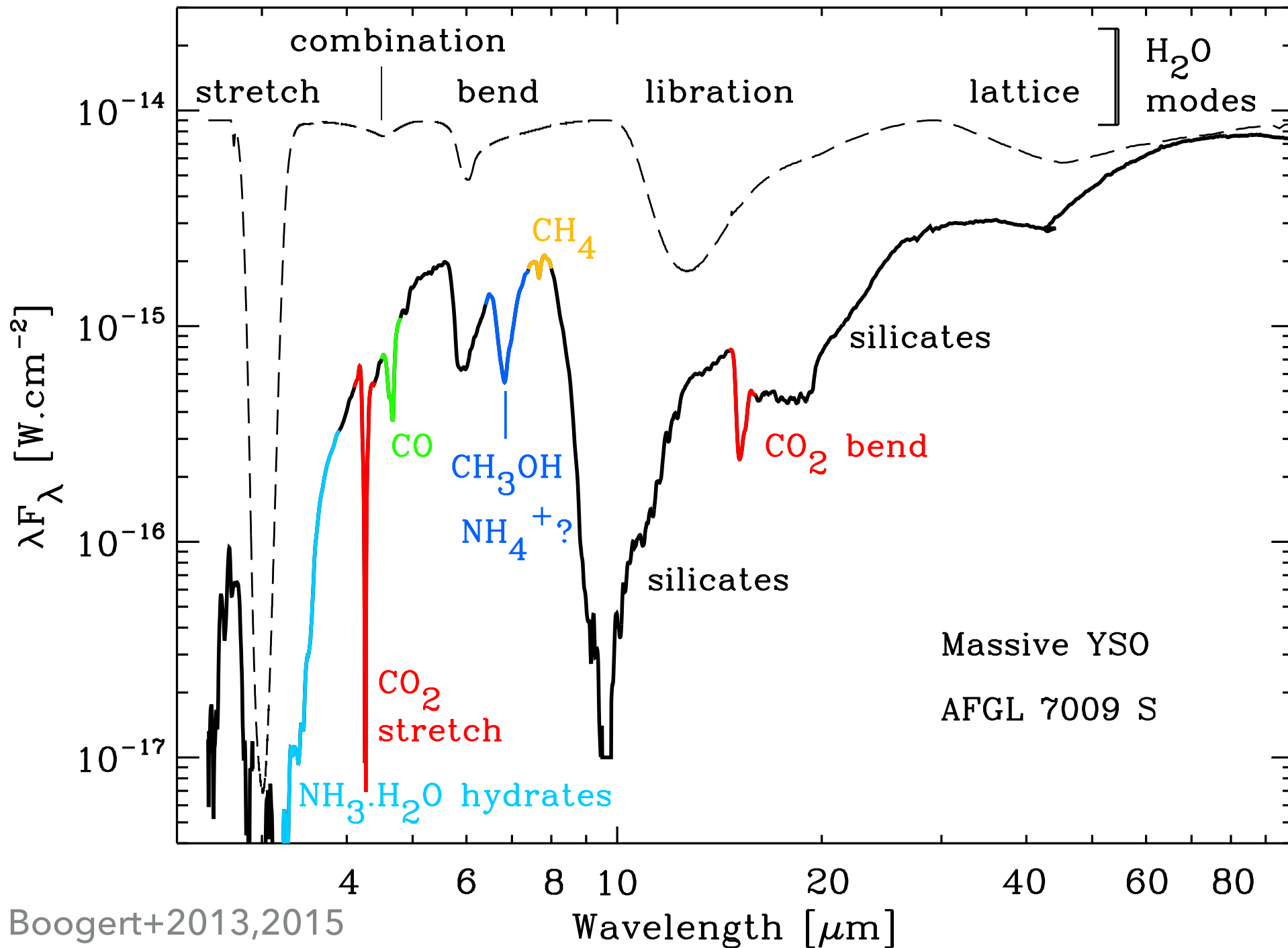
Spitzer Space Telescope (High-sensitivity) Ices, silicates, PAHs

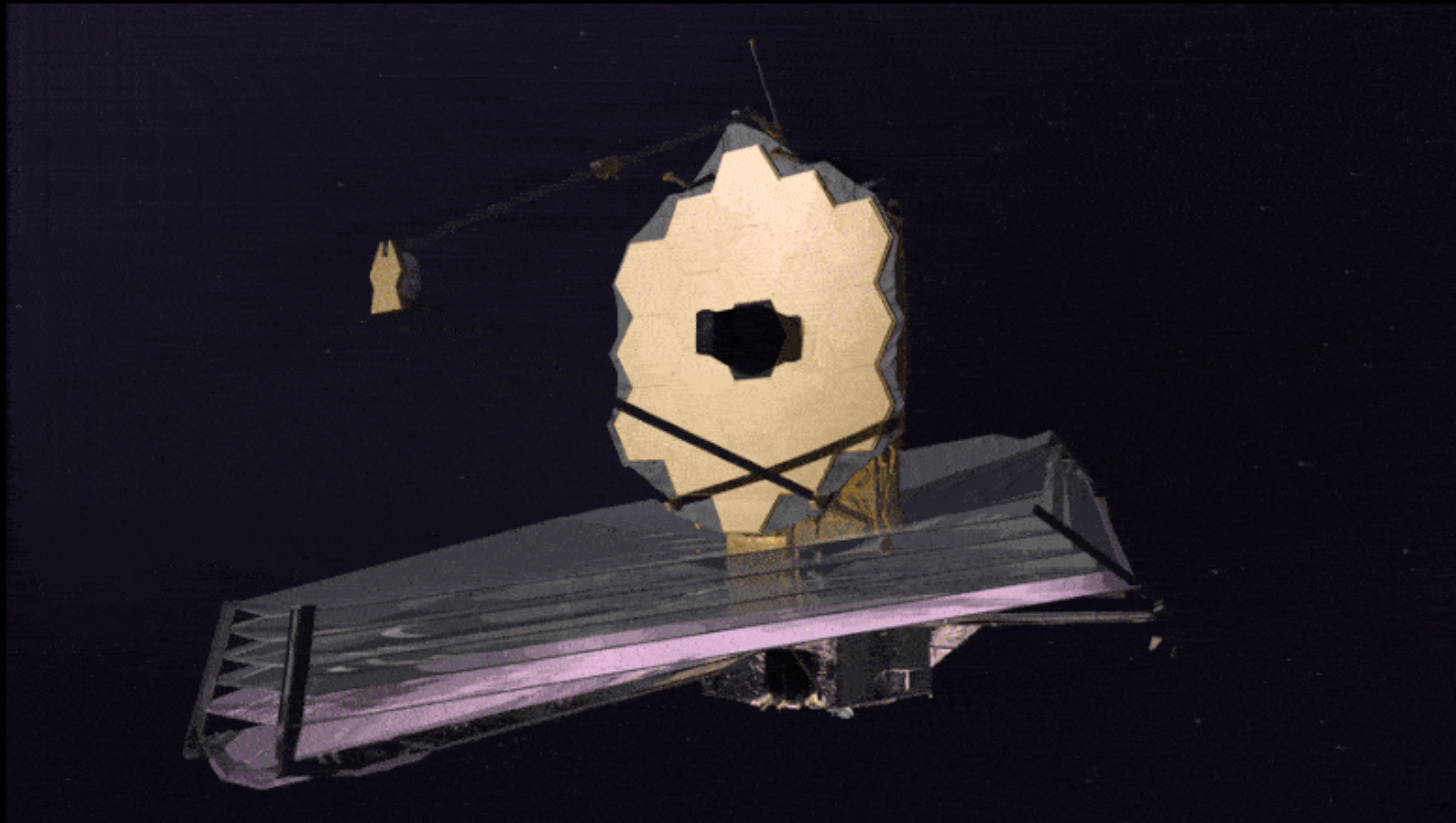


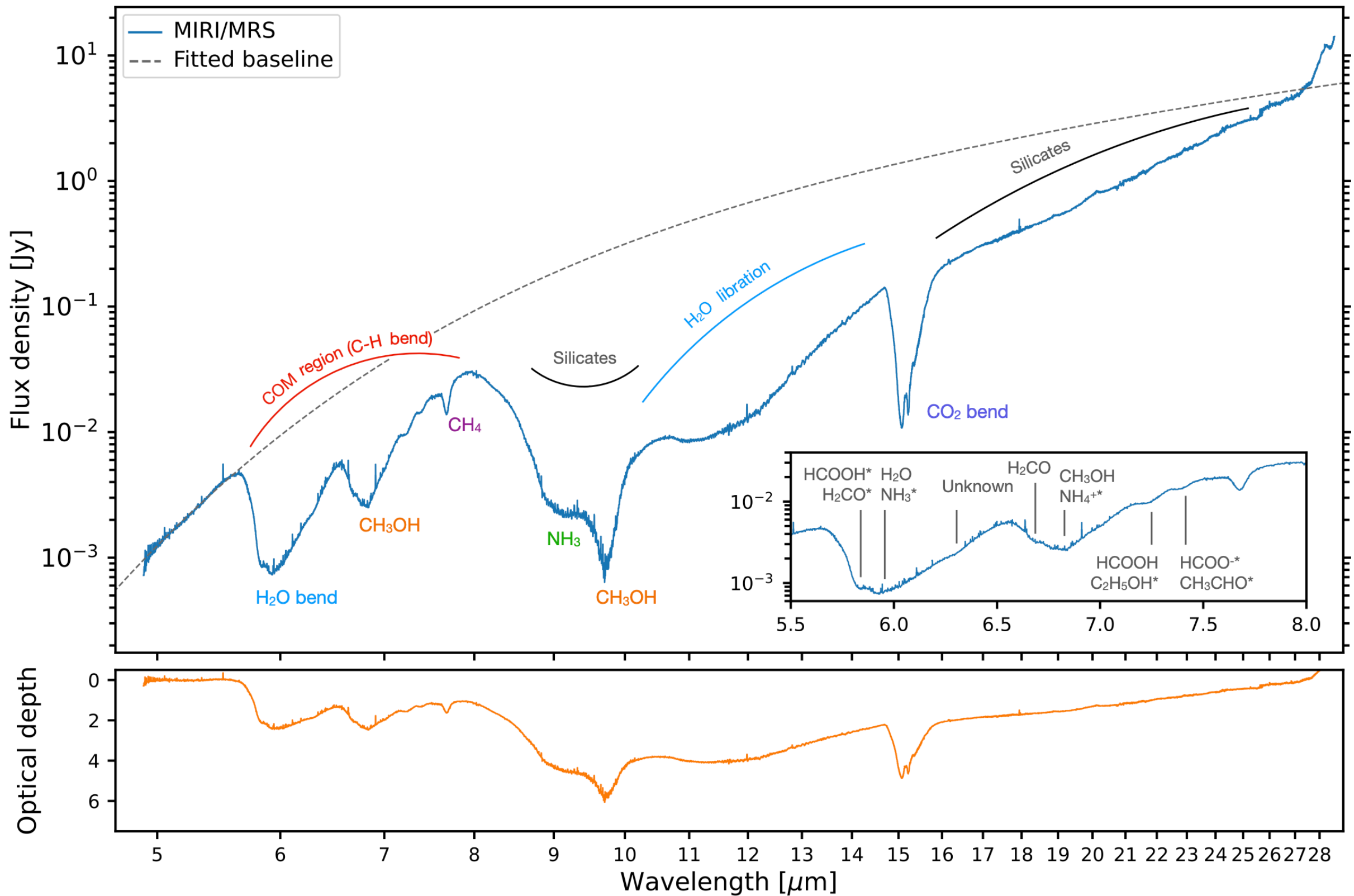


# THE MOLECULAR UNIVERSE TIMELINE

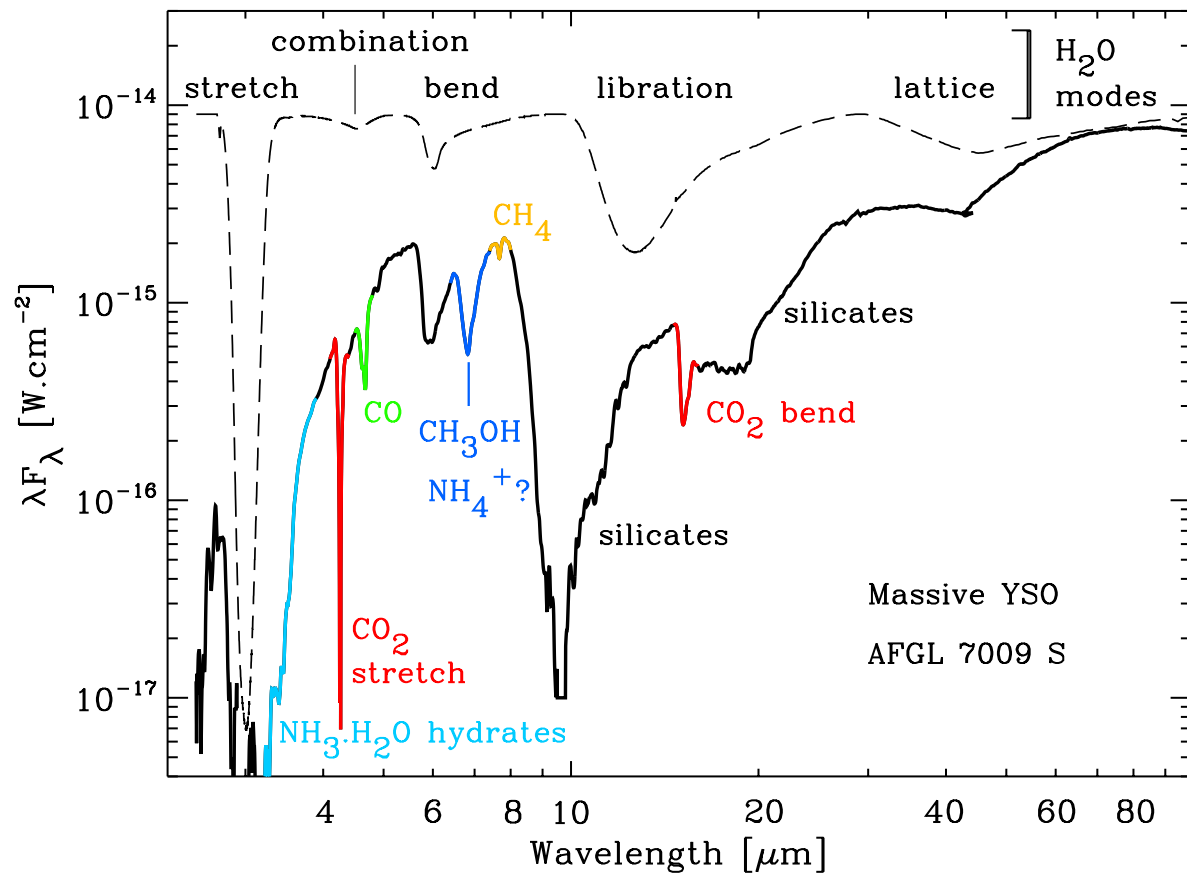
## INVENTORY OF ICES







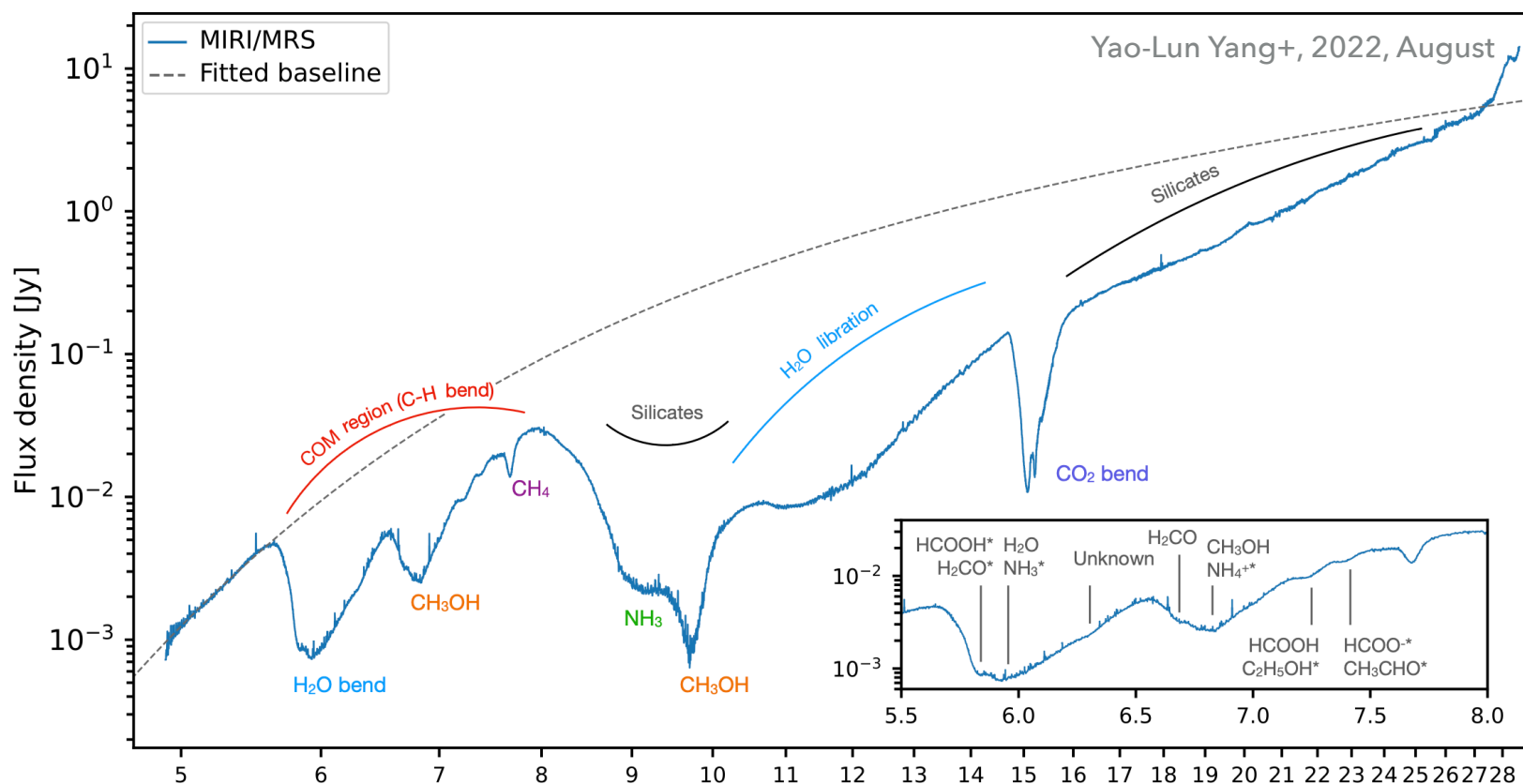




They confirmed some of the laboratory and observational work



They also found some new interesting features @6.31 and 7.24 micron

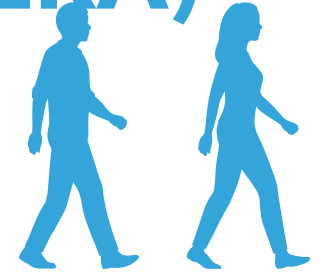


**Table 1.** Notable ice features

Wavelength ( $\mu\text{m}$ )	Type	Identification
5.83	single	$\text{HCOOH}^*$ , $\text{H}_2\text{CO}^*$
6	multiple	$\text{H}_2\text{O}$ , $\text{NH}_3^*$
6.31	single	unknown
6.7	single	$\text{H}_2\text{CO}$
6.8	multiple	$\text{CH}_3\text{OH}$ , $\text{NH}_4^{+*}$
7.24	single	$\text{HCOOH}$ , $\text{C}_2\text{H}_5\text{OH}^*$
7.41	single	$\text{HCOO}^-*$ , $\text{CH}_3\text{CHO}^*$
7.7	single	$\text{CH}_4$ , $\text{SO}_2^*$ , $\text{C}_2\text{H}_5\text{OH}^*$
9	single	$\text{NH}_3$ , $\text{CH}_3\text{OH}^*$ , $\text{C}_2\text{H}_5\text{OH}^*$
9.7	single	$\text{CH}_3\text{OH}$
11	single/broad	$\text{H}_2\text{O}$ , $\text{C}_2\text{H}_5\text{OH}^*$ , $\text{CH}_3\text{CHO}^*$ , $\text{HCOOCH}_3^*$
15.2	multiple	$\text{CO}_2$

\*Potential/ambiguous identification

# THE MOLECULAR UNIVERSE TIMELINE (ALMA ERA)



2004

ALMA CONSTRUCTION STARTED

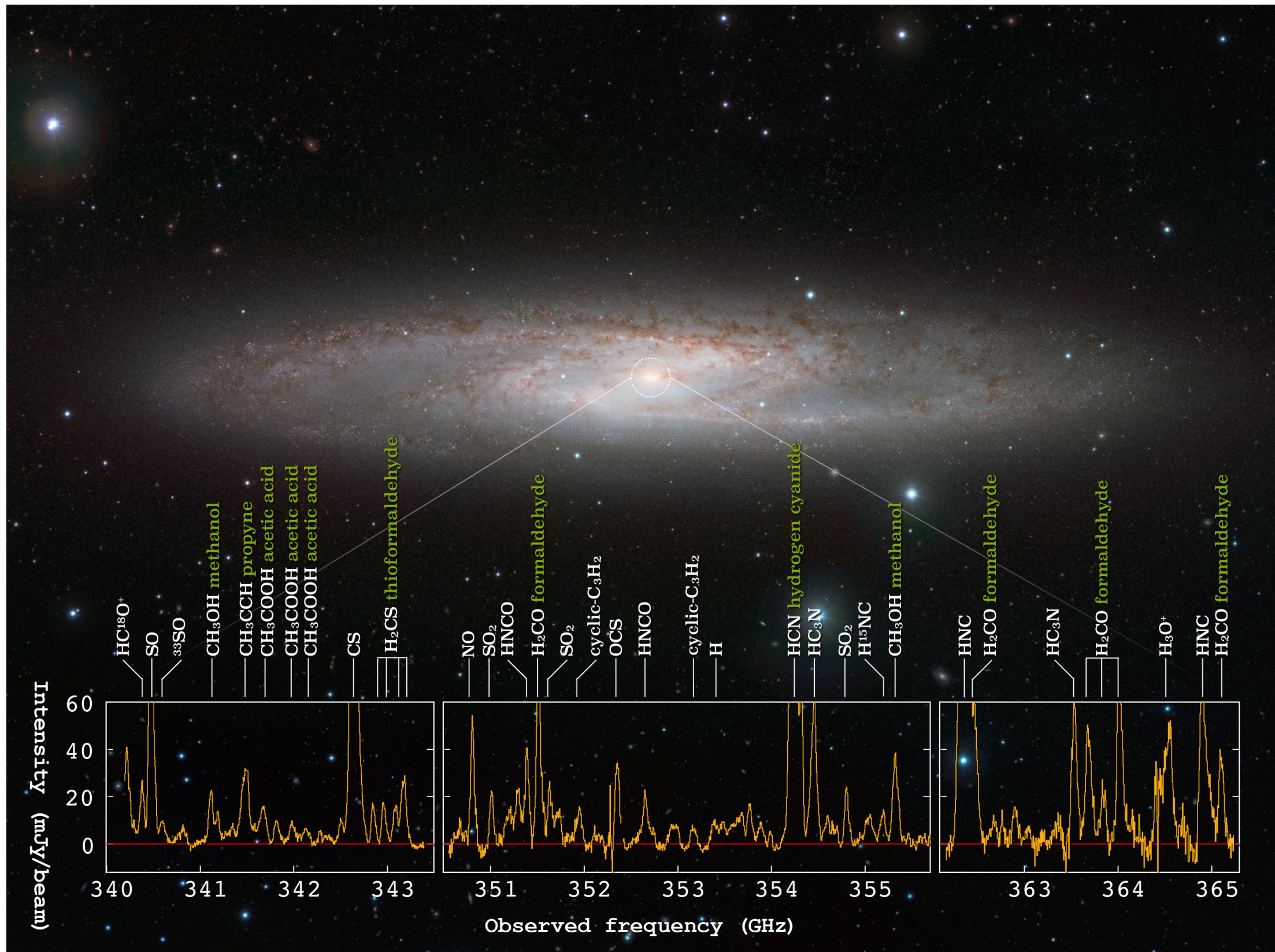
**Established Astrochemistry**



2018

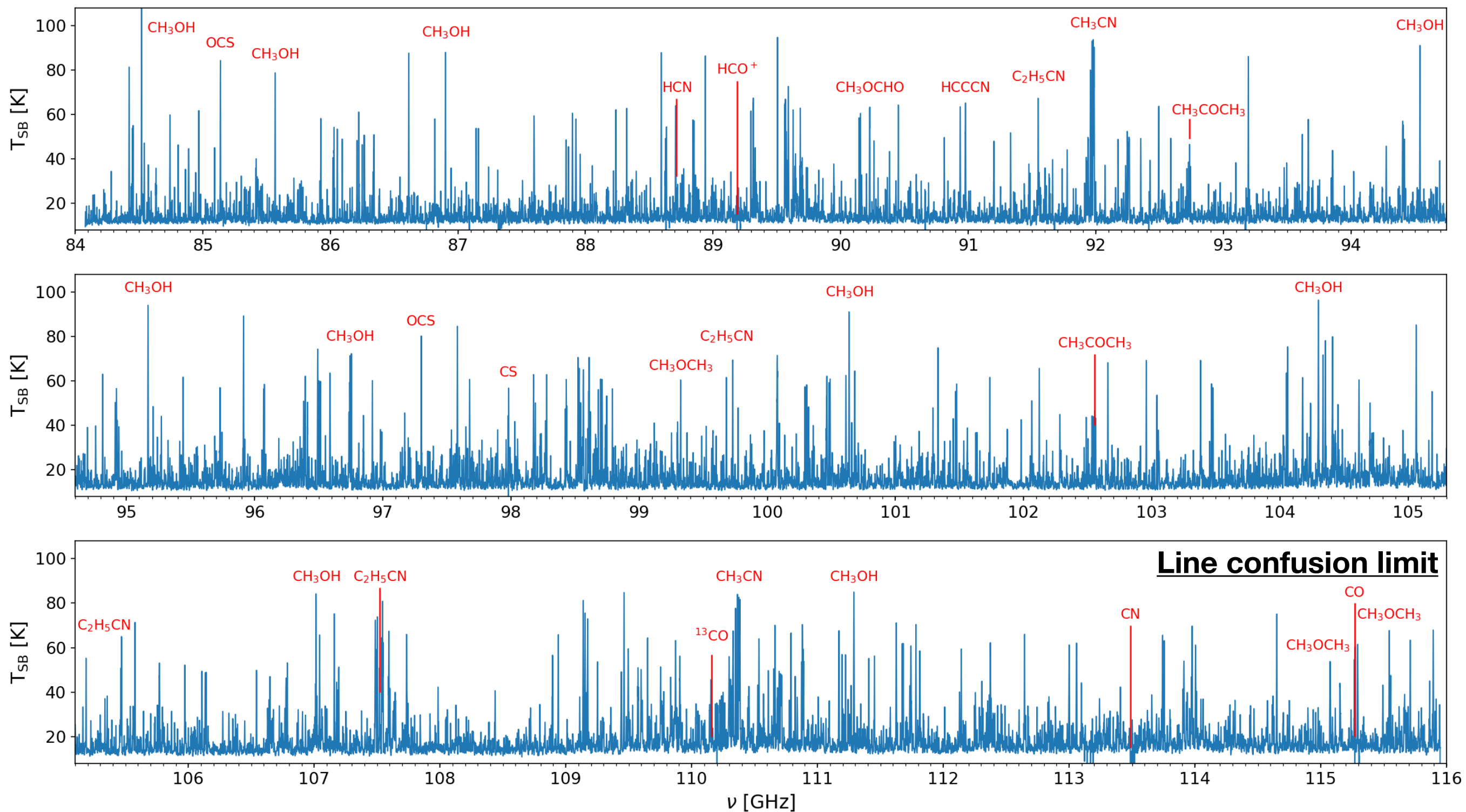
~ 200 molecules have been detected (not counting isotopes)  
(<https://www.astro.uni-koeln.de/cdms/molecules>)





~ 200 molecules have been detected (not counting isotopes)  
<https://www.astro.uni-koeln.de/cdms/molecules>



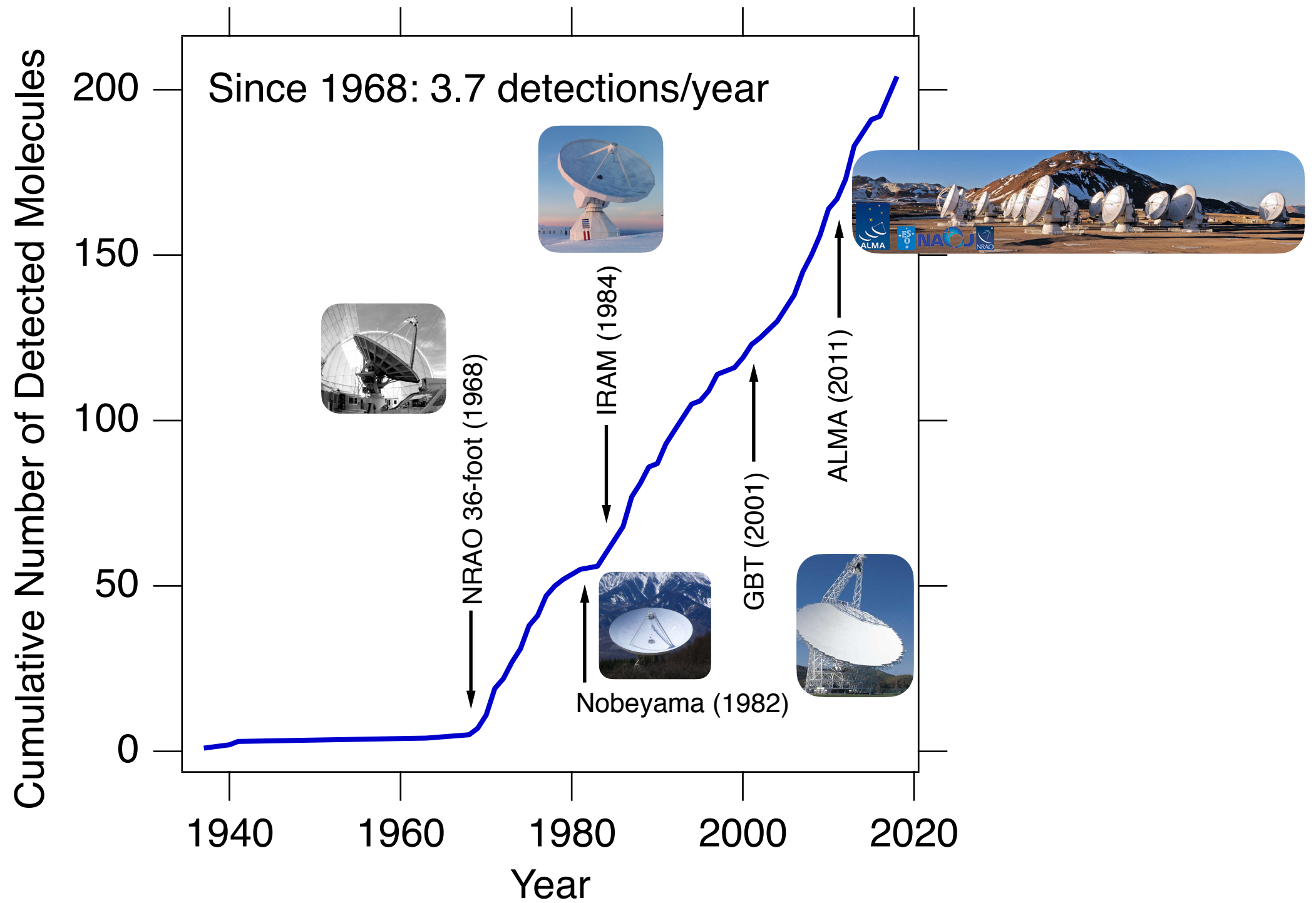


# HTTPS://CDMS.ASTRO.UNI-KOELN.DE/CLASSIC/MOLECULES

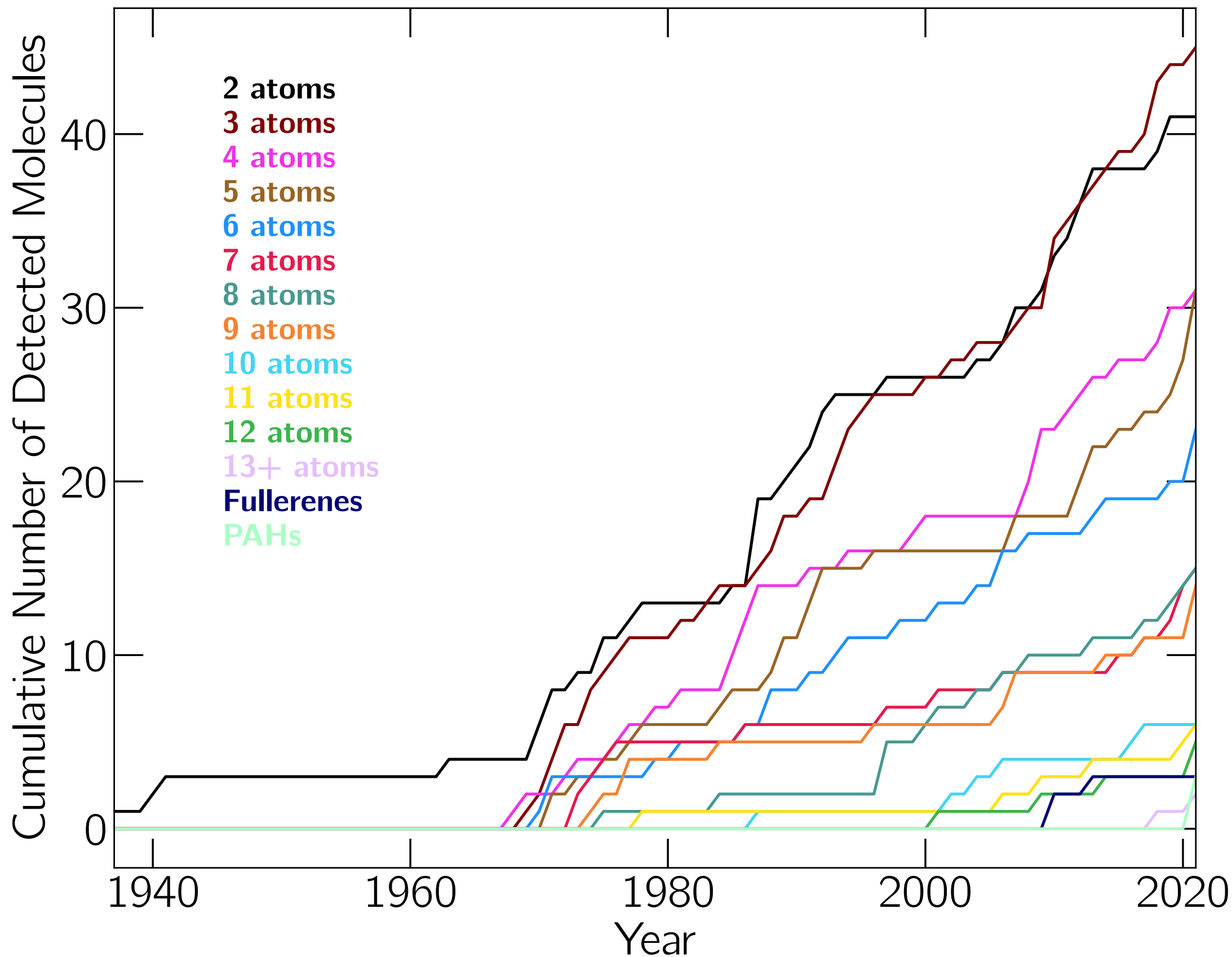
## Molecules in the Interstellar Medium or Circumstellar Shells (as of 03/2018)

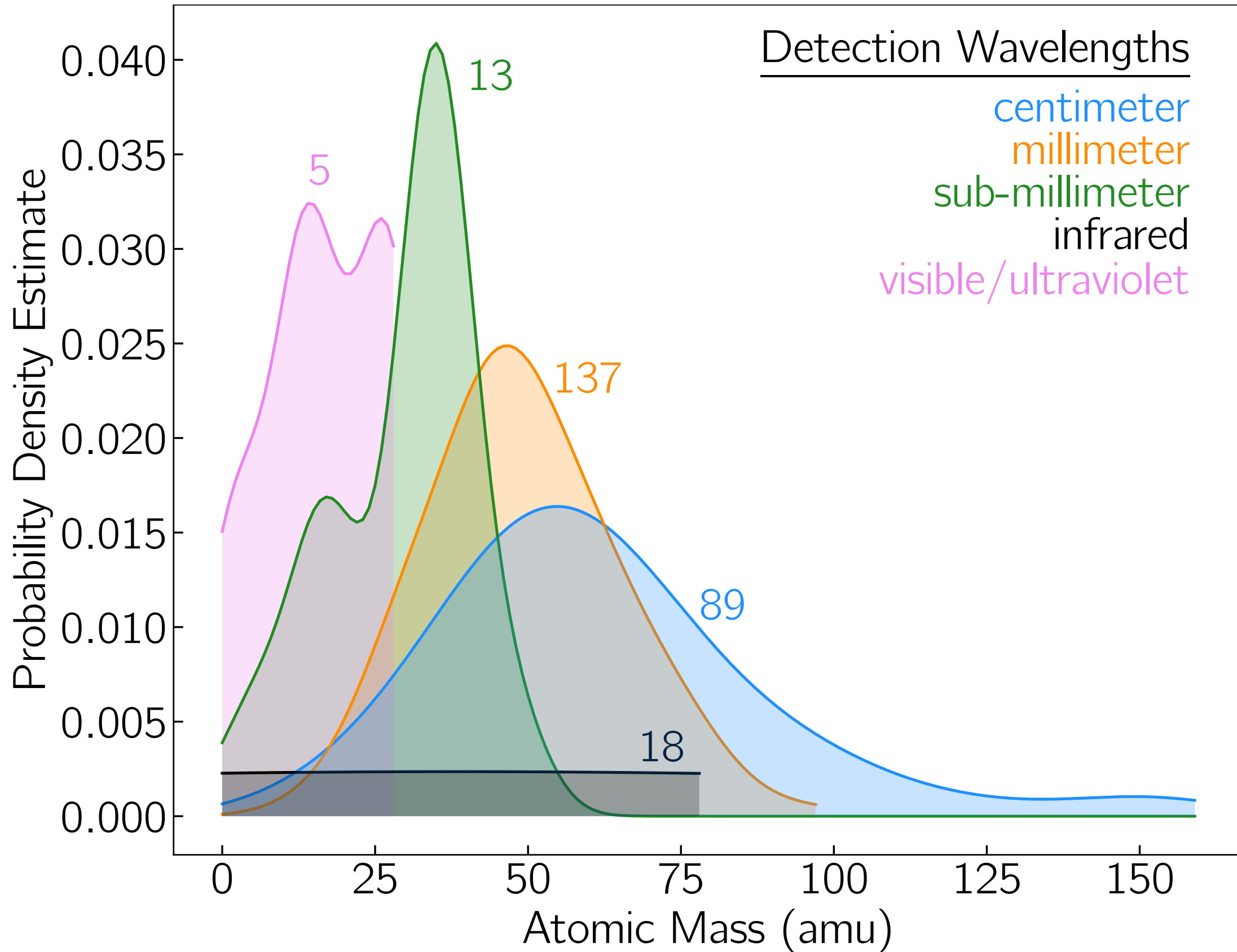
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
H <sub>2</sub>	C <sub>3</sub> <sup>*</sup>	<i>c</i> -C <sub>3</sub> H	C <sub>5</sub> <sup>*</sup>	C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> C <sub>5</sub> N	HC <sub>9</sub> N	<i>c</i> -C <sub>6</sub> H <sub>6</sub> <sup>*</sup>	C <sub>60</sub> <sup>*</sup>
AlF	C <sub>2</sub> H	<i>l</i> -C <sub>3</sub> H	C <sub>4</sub> H	<i>l</i> -H <sub>2</sub> C <sub>4</sub>	CH <sub>2</sub> CHCN	HC(O)OCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>3</sub> ) <sub>2</sub> CO	CH <sub>3</sub> C <sub>6</sub> H	<i>n</i> -C <sub>3</sub> H <sub>7</sub> CN	C <sub>70</sub> <sup>*</sup>
AlCl	C <sub>2</sub> O	C <sub>3</sub> N	C <sub>4</sub> Si	C <sub>2</sub> H <sub>4</sub> <sup>*</sup>	CH <sub>3</sub> C <sub>2</sub> H	CH <sub>3</sub> COOH	(CH <sub>3</sub> ) <sub>2</sub> O	(CH <sub>2</sub> OH) <sub>2</sub>	C <sub>2</sub> H <sub>5</sub> OCHO	<i>i</i> -C <sub>3</sub> H <sub>7</sub> CN	C <sub>60</sub> <sup>+</sup> <sup>*</sup>
C <sub>2</sub> <sup>**</sup>	C <sub>2</sub> S	C <sub>3</sub> O	<i>l</i> -C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> CN	HC <sub>5</sub> N	C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> CH <sub>2</sub> CHO	CH <sub>3</sub> OC(O)CH <sub>3</sub>	C <sub>2</sub> H <sub>5</sub> OCH <sub>3</sub> <sup>?</sup>	<i>c</i> -C <sub>6</sub> H <sub>5</sub> CN 2018
CH	CH <sub>2</sub>	C <sub>3</sub> S	<i>c</i> -C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> NC	CH <sub>3</sub> CHO	C <sub>6</sub> H <sub>2</sub>	HC <sub>7</sub> N	CH <sub>3</sub> CHCH <sub>2</sub> O 2016			
CH <sup>+</sup>	HCN	C <sub>2</sub> H <sub>2</sub> <sup>*</sup>	H <sub>2</sub> CCN	CH <sub>3</sub> OH	CH <sub>3</sub> NH <sub>2</sub>	CH <sub>2</sub> OHCHO	C <sub>8</sub> H	CH <sub>3</sub> OCH <sub>2</sub> OH 2017			
CN	HCO	NH <sub>3</sub>	CH <sub>4</sub> <sup>*</sup>	CH <sub>3</sub> SH	<i>c</i> -C <sub>2</sub> H <sub>4</sub> O	<i>l</i> -HC <sub>6</sub> H <sup>*</sup>	CH <sub>3</sub> C(O)NH <sub>2</sub>				
CO	HCO <sup>+</sup>	HCCN	HC <sub>3</sub> N	HC <sub>3</sub> NH <sup>+</sup>	H <sub>2</sub> CCHOH	CH <sub>2</sub> CHCHO(?)	C <sub>8</sub> H <sup>-</sup>				
CO <sup>+</sup>	HCS <sup>+</sup>	HCNH <sup>+</sup>	HC <sub>2</sub> NC	HC <sub>2</sub> CHO	C <sub>6</sub> H <sup>-</sup>	CH <sub>2</sub> CCHCN	C <sub>3</sub> H <sub>6</sub>				
CP	HOC <sup>+</sup>	HNCO	HCOOH	NH <sub>2</sub> CHO	CH <sub>3</sub> NCO	H <sub>2</sub> NCH <sub>2</sub> CN	CH <sub>3</sub> CH <sub>2</sub> SH(?)				
SiC	H <sub>2</sub> O	HNCS	H <sub>2</sub> CNH	C <sub>5</sub> N	HC <sub>5</sub> O 2017	CH <sub>3</sub> CHNH	CH <sub>3</sub> NHCHO? 2017				
HCl	H <sub>2</sub> S	HOCO <sup>+</sup>	H <sub>2</sub> C <sub>2</sub> O	<i>l</i> -HC <sub>4</sub> H <sup>*</sup>		CH <sub>3</sub> SiH <sub>3</sub> 2017	HC <sub>7</sub> O 2017				
KCl	HNC	H <sub>2</sub> CO	H <sub>2</sub> NCN	<i>l</i> -HC <sub>4</sub> N							
NH	HNO	H <sub>2</sub> CN	HNC <sub>3</sub>	<i>c</i> -H <sub>2</sub> C <sub>3</sub> O							
NO	MgCN	H <sub>2</sub> CS	SiH <sub>4</sub> <sup>*</sup>	H <sub>2</sub> CCNH(?)							
NS	MgNC	H <sub>3</sub> O <sup>+</sup>	H <sub>2</sub> COH <sup>+</sup>	C <sub>5</sub> N <sup>-</sup>							
NaCl	N <sub>2</sub> H <sup>+</sup>	<i>c</i> -SiC <sub>3</sub>	C <sub>4</sub> H <sup>-</sup>	HNCHCN							
OH	N <sub>2</sub> O	CH <sub>3</sub> <sup>*</sup>	HC(O)CN	SiH <sub>3</sub> CN 2017							
PN	NaCN	C <sub>3</sub> N <sup>-</sup>	HNCNH								
SO	OCS	PH <sub>3</sub>	CH <sub>3</sub> O								
SO <sup>+</sup>	SO <sub>2</sub>	HCNO	NH <sub>4</sub> <sup>+</sup>								

INCOMPLETE



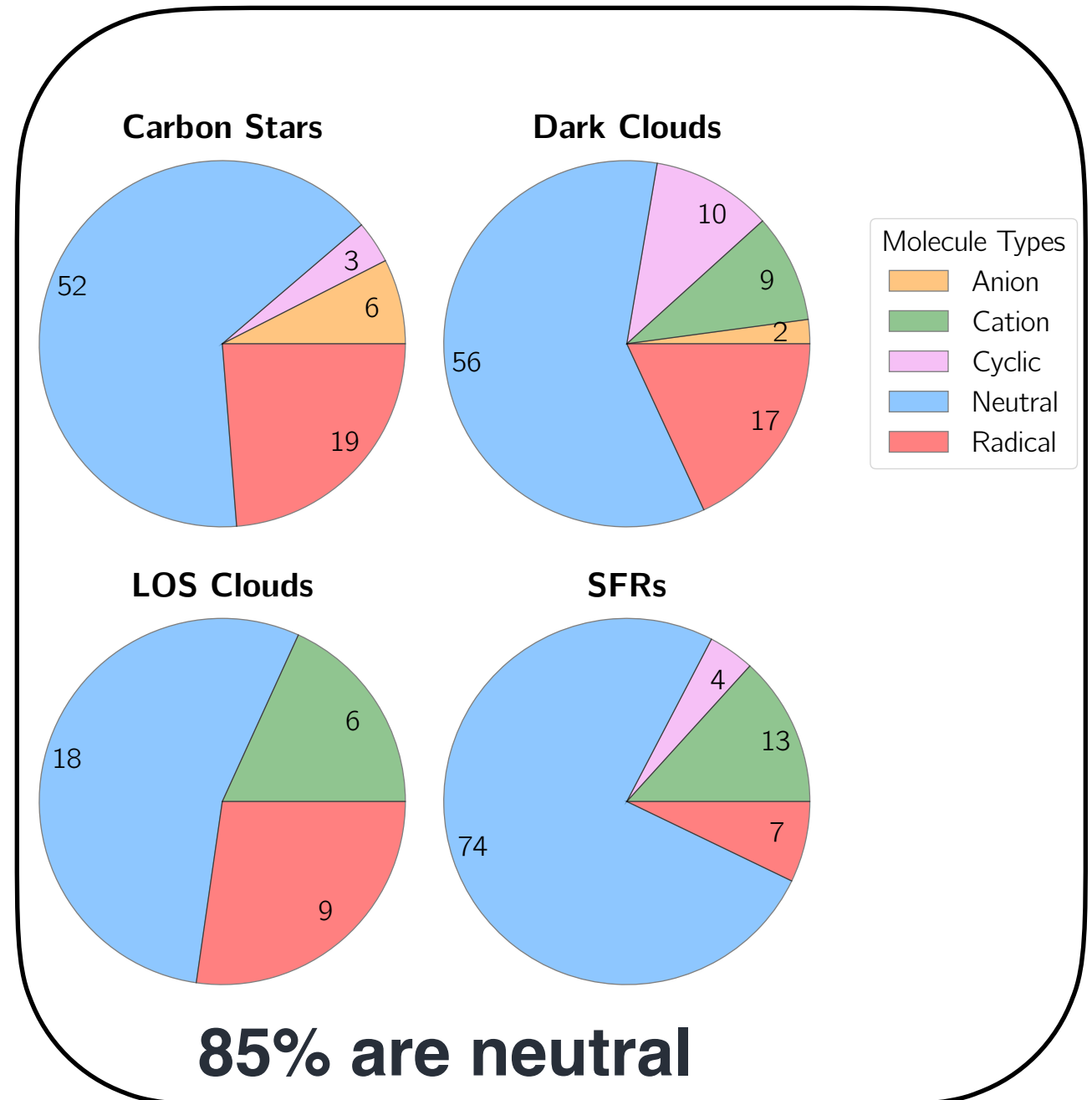
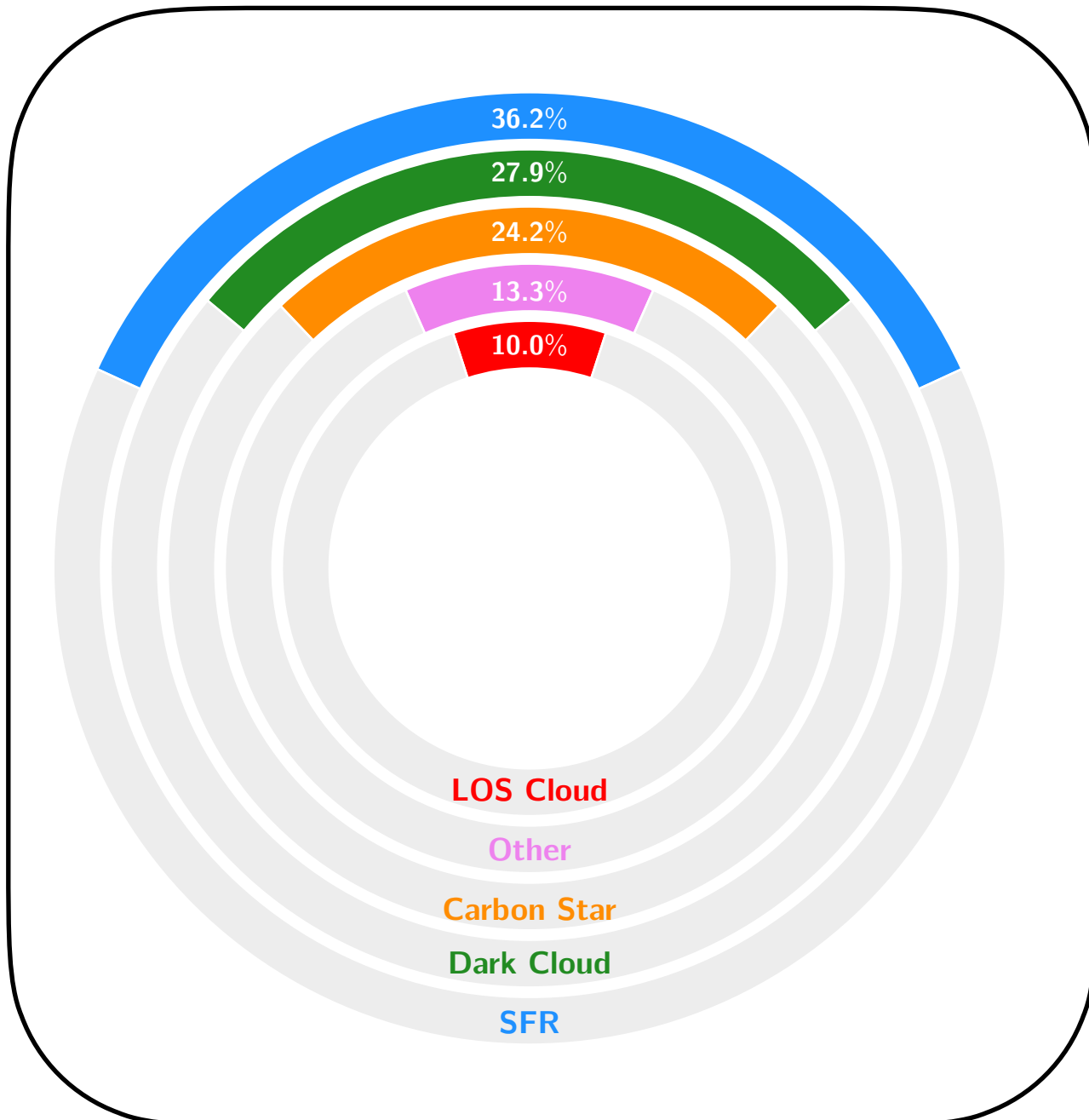






# Where most of the molecules are

More than 50% of molecules observed in dark clouds and SFR



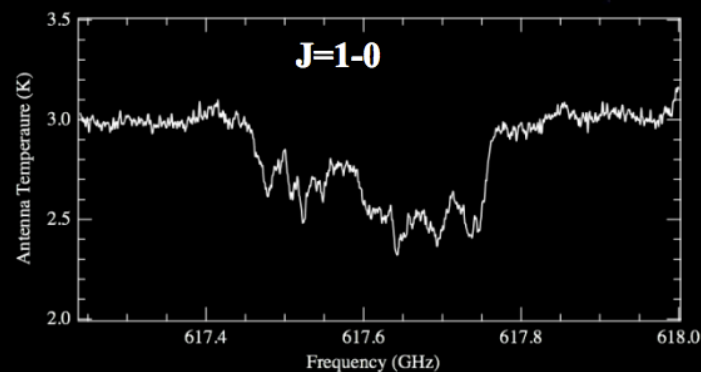


# First interstellar noble gas molecule!

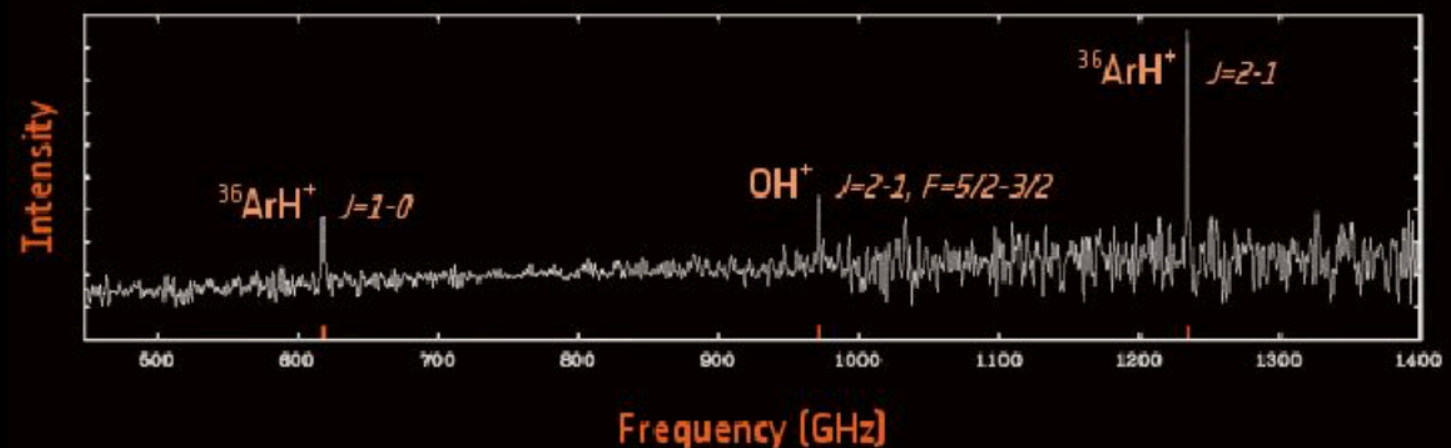


Crab nebula  
Hubble+ Herschel

Barlow et al. 2013  
Herschel-SPIRE

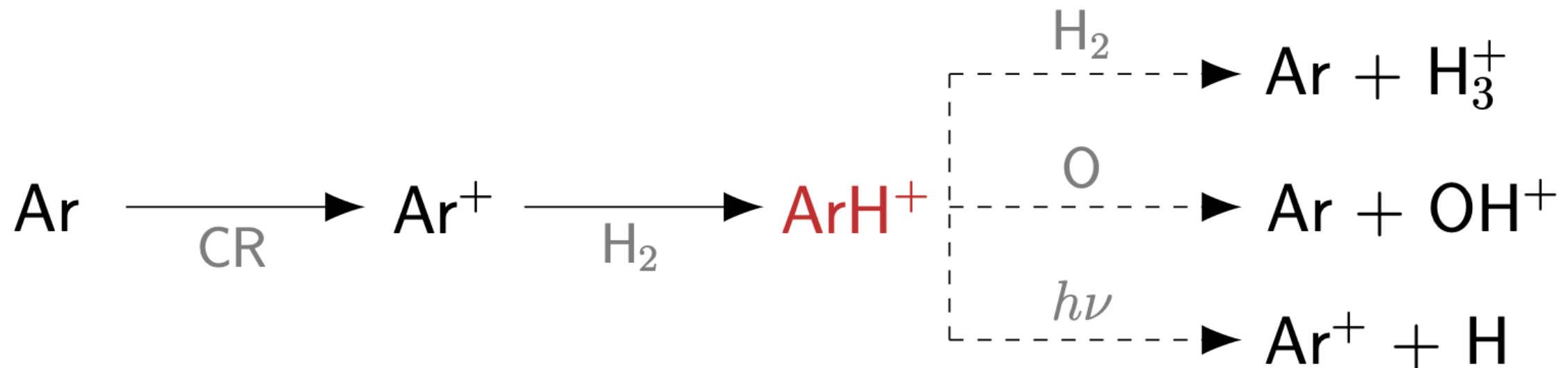


Schilke et al. 2014  
Herschel-HIFI Sgr B2



# FIRST INTERSTELLAR NOBLE GAS MOLECULE

Jacob+2022



- ▶ 617 GHz absorption line identified by Barlow+2013
- ▶ A molecule which traces purely atomic gas (diffuse,  $f(\text{H}_2) \sim 10^{-4} - 10^{-2}$ )
- ▶ It is a tracer of cosmic-rays (very reliable)

# Astromolecule of the Month

January 2016



HeH<sup>+</sup>

The helium hydride ion, HeH<sup>+</sup>, is thought to be involved in some of the earliest chemistry to occur in the universe, formed through the **radiative association** reaction



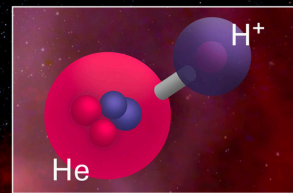
In fact, recent calculations by **Bovino et al.** indicate that its abundance in the early universe may have been 10 times greater than previously thought.

Since HeH<sup>+</sup> is readily destroyed by reactions with most neutral species, it has proven difficult to detect it in the modern era. The most recent effort was a search for the  $J=1-0$  transition toward a high redshift **quasar** by **Zinchenko et al.** in 2011. While they observed something very weak shifted slightly from the expected frequency, the weakness, narrow linewidth, and anomalous velocity cast of the feature doubt that it is due to HeH<sup>+</sup>. Previously, **Liu et al.** had unsuccessfully sought for HeH<sup>+</sup> toward the **planetary nebula NGC 7027**.

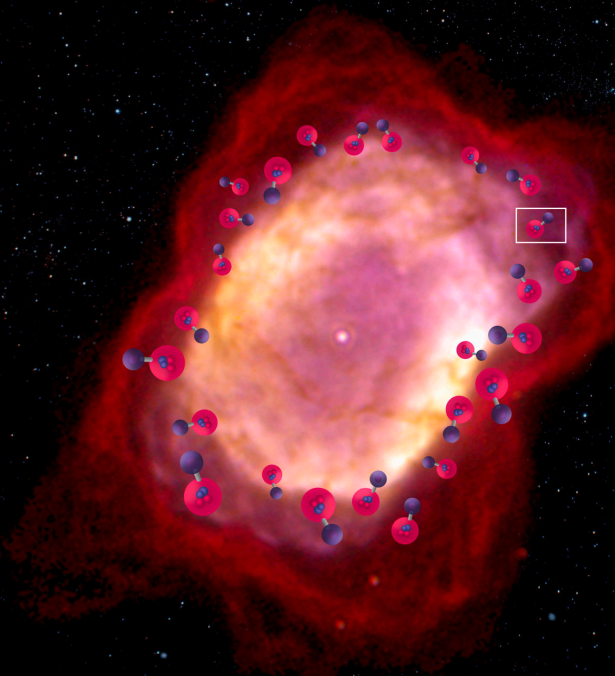
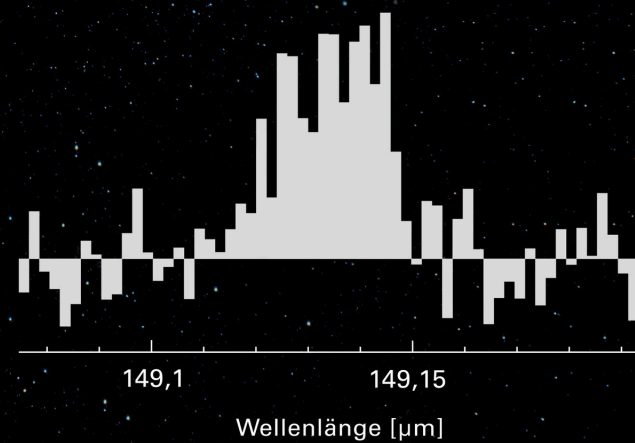


Güsten+2019

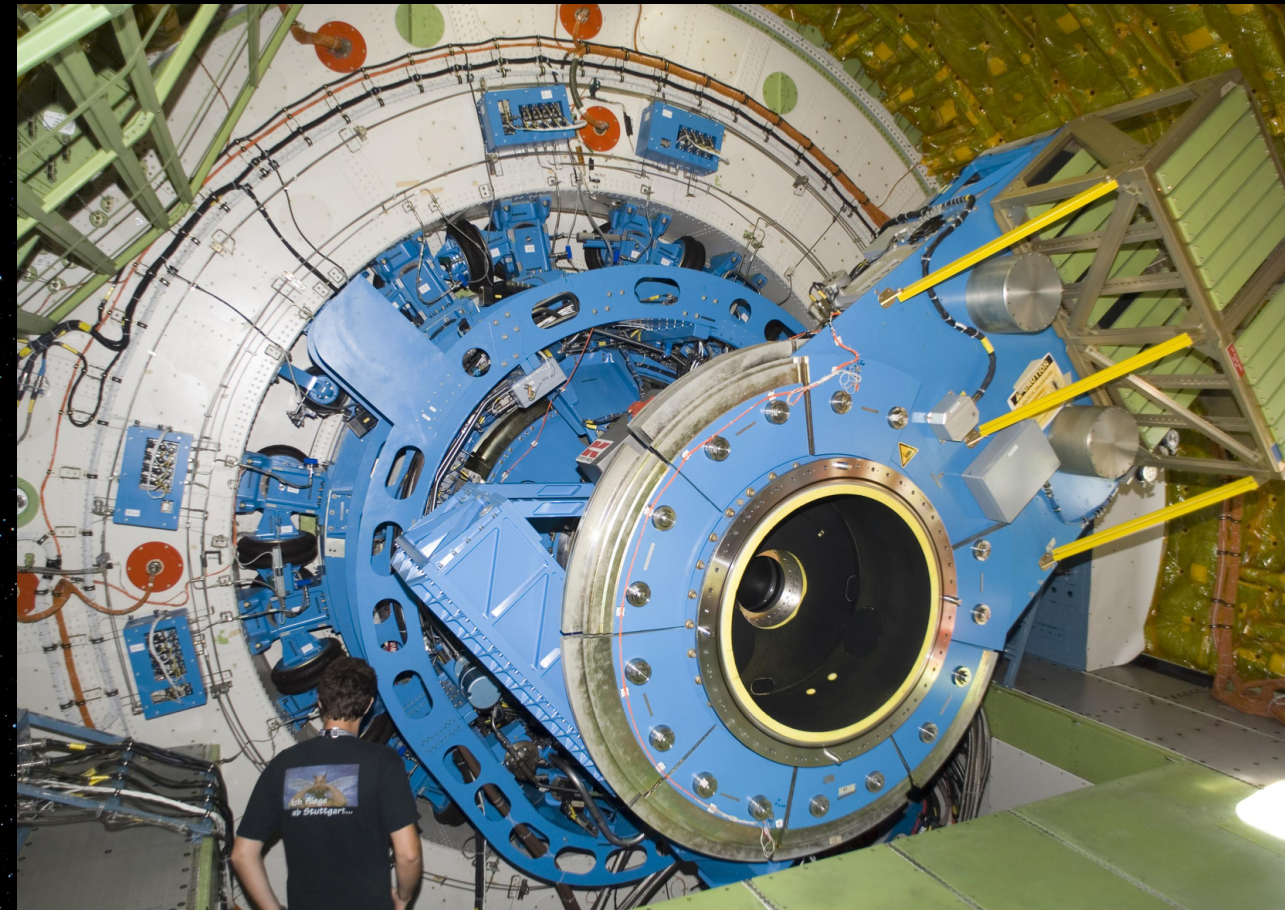
Heliumhydrid in NGC 7027 entdeckt



HeH<sup>+</sup> J=1→0



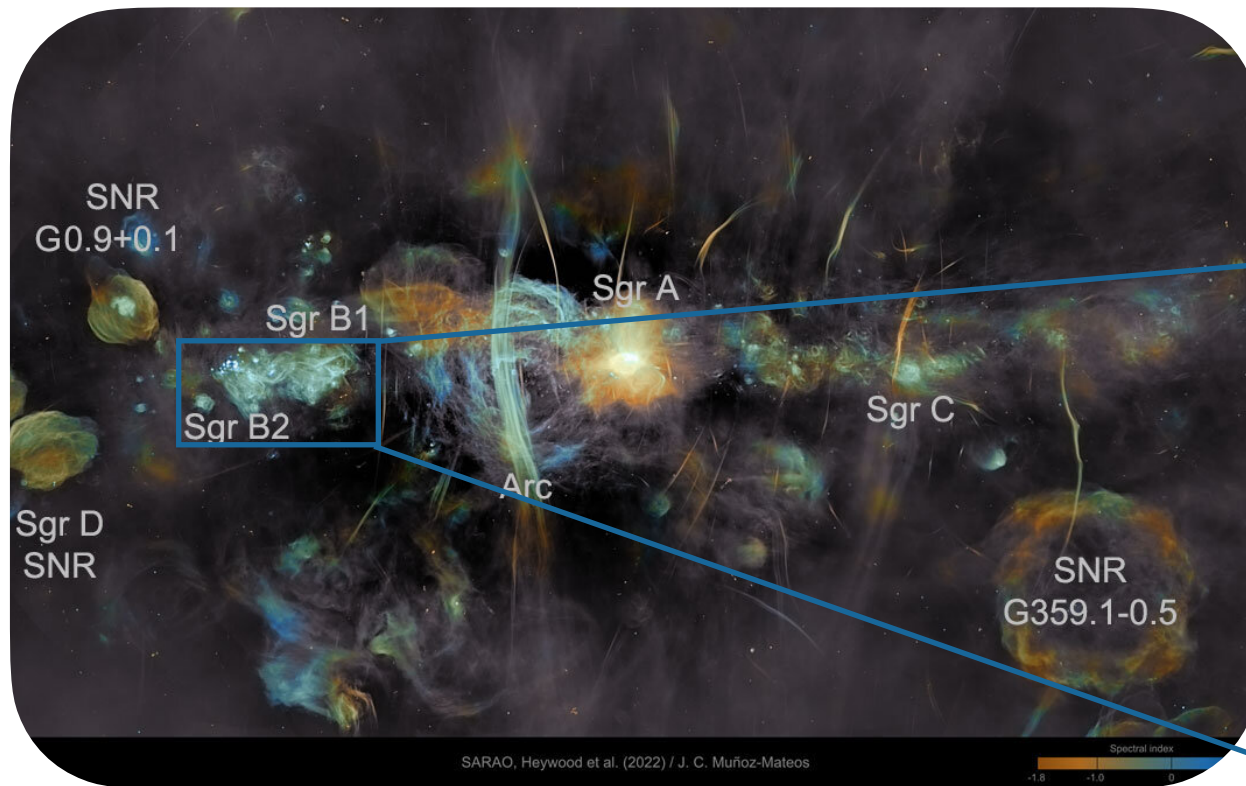
Observed with SOFIA in a planetary nebula



**SECOND INTERSTELLAR NOBLE GAS MOLECULE**



# SAGITTARIUS B2: COMPLEX ORGANIC MOLECULES



GMC @ 120 pc from the center of the MW



One of the largest GMC in our galaxy ( $M \sim 3 \times 10^6 M_{\text{sun}}$ )

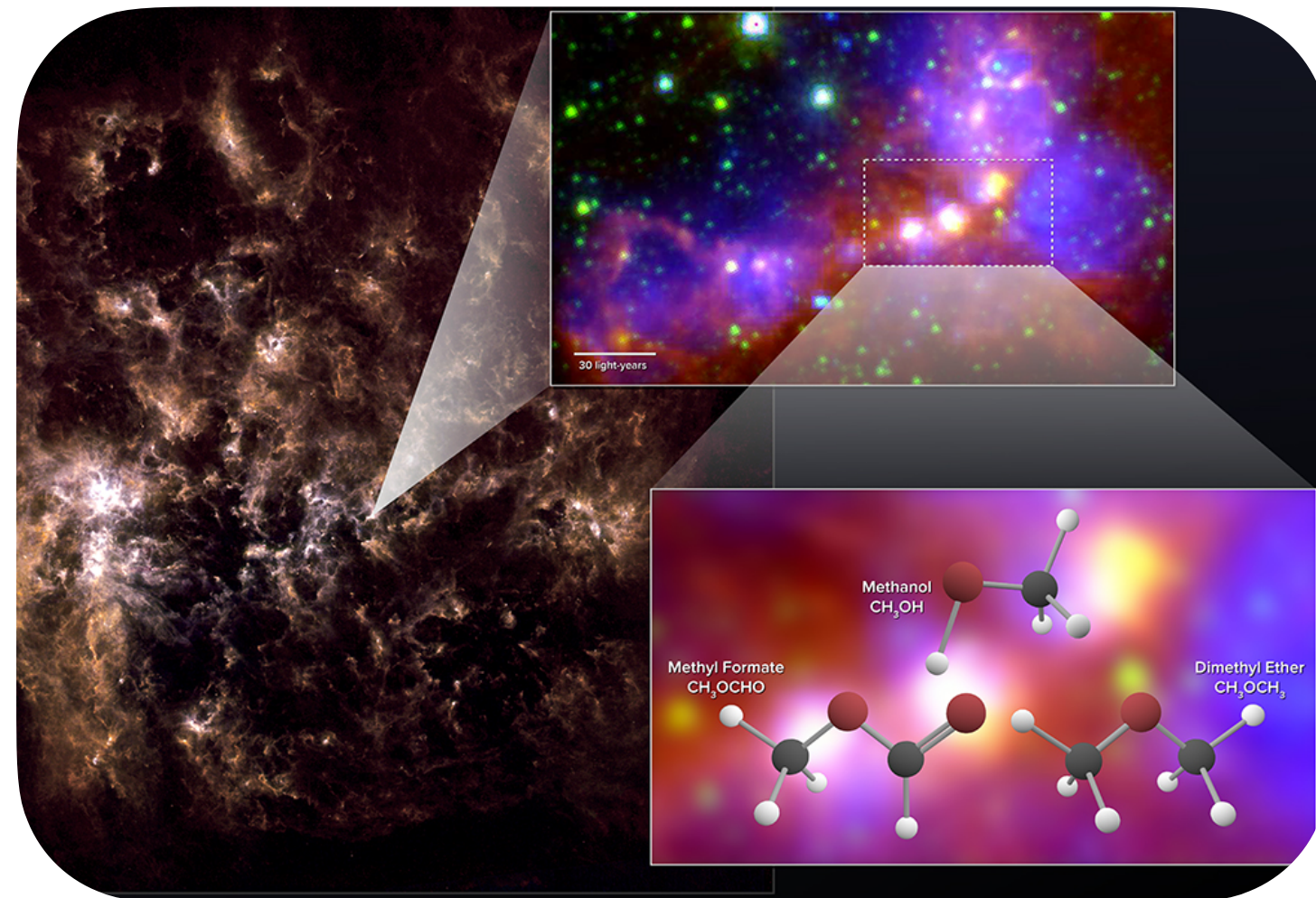
**It is well known for tasting like raspberries and smelling like rum!**

It contains ethyl formate which is an ester known for tasting like raspberries.

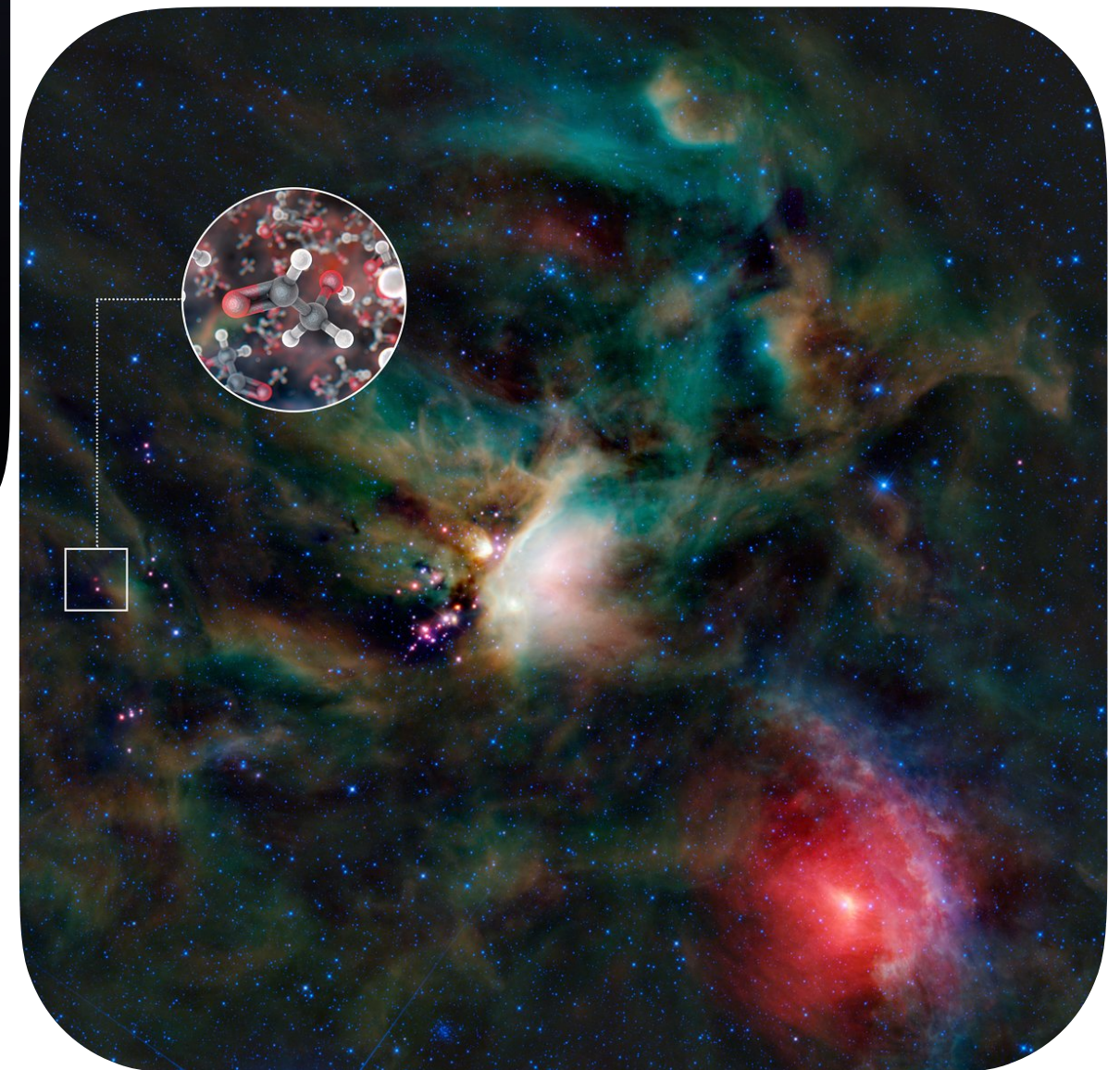
It also contains enough ethanol for each person on earth to drink 300,000 pintes a day for a billion years.



# COMPLEX ORGANIC MOLECULES



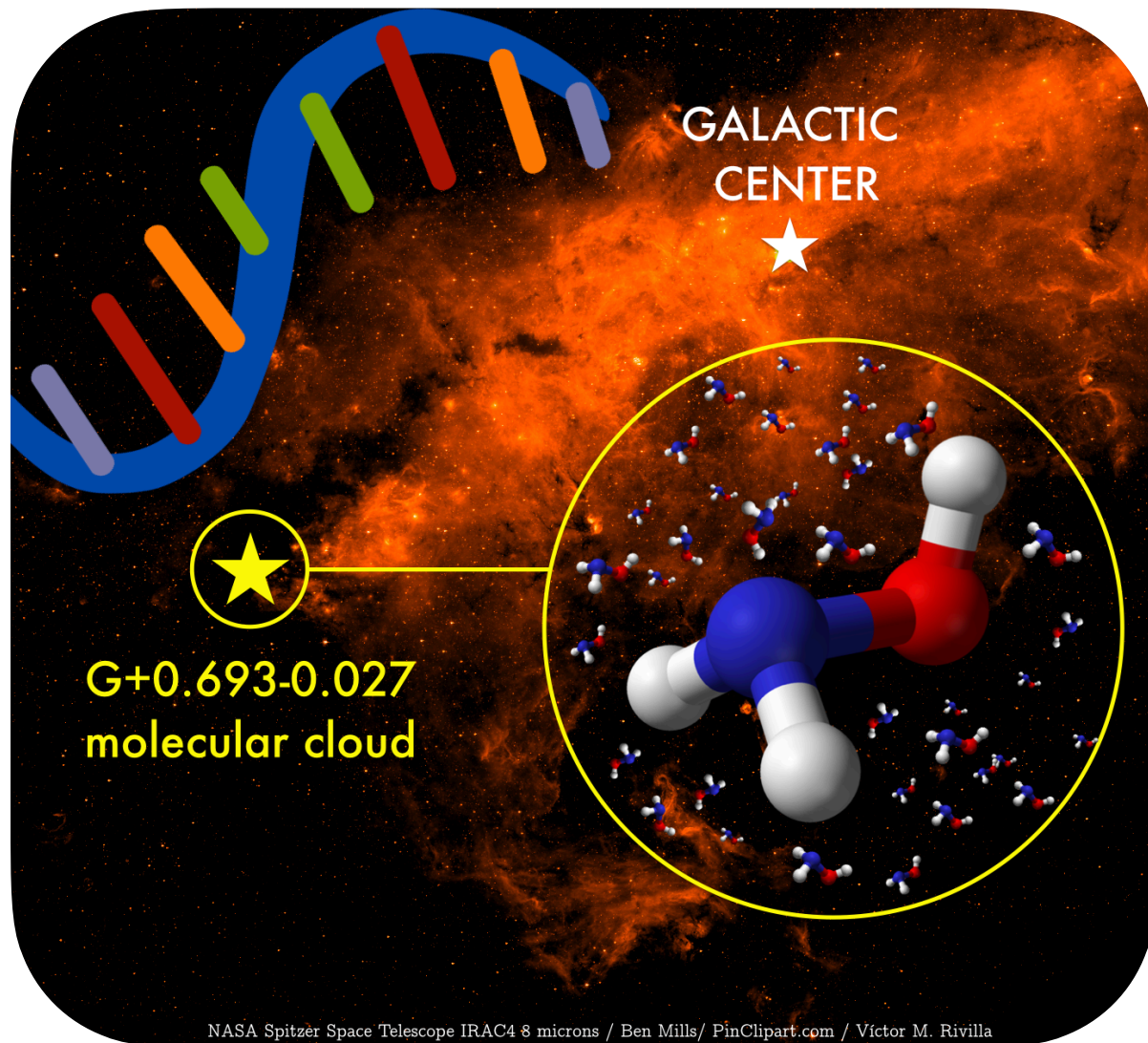
Glycolaldehyde: observed close to a star similar to our Sun (the simplest molecules related to sugars).



- Hydrogen (H)
- Carbon (C)
- Oxygen (O)

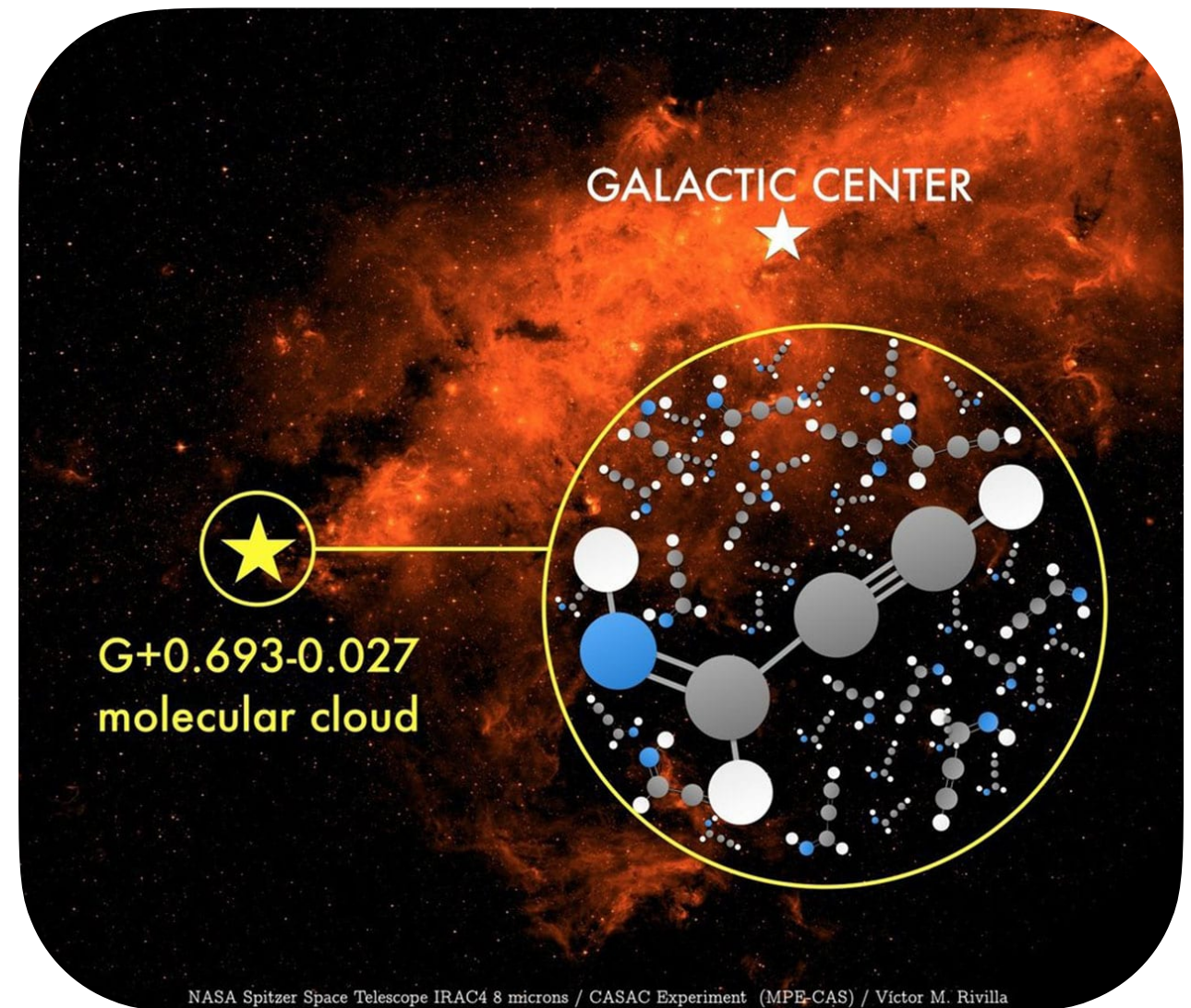
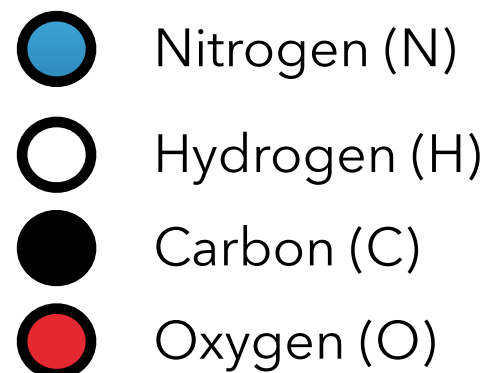


# COMPLEX ORGANIC MOLECULES



Hydroxylamine

Precursor of RNA

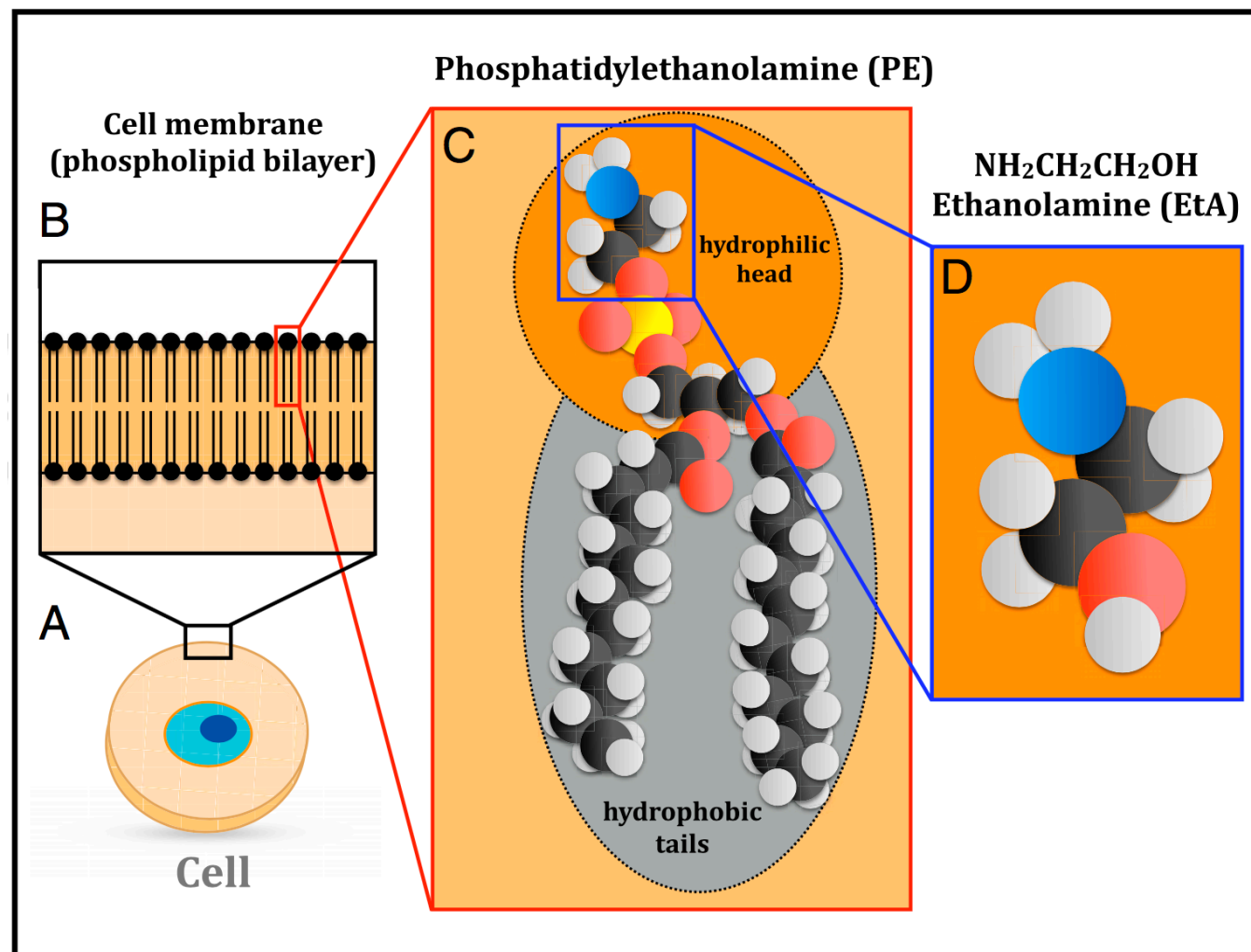


Propargylimine

Building block of  
amino-acid

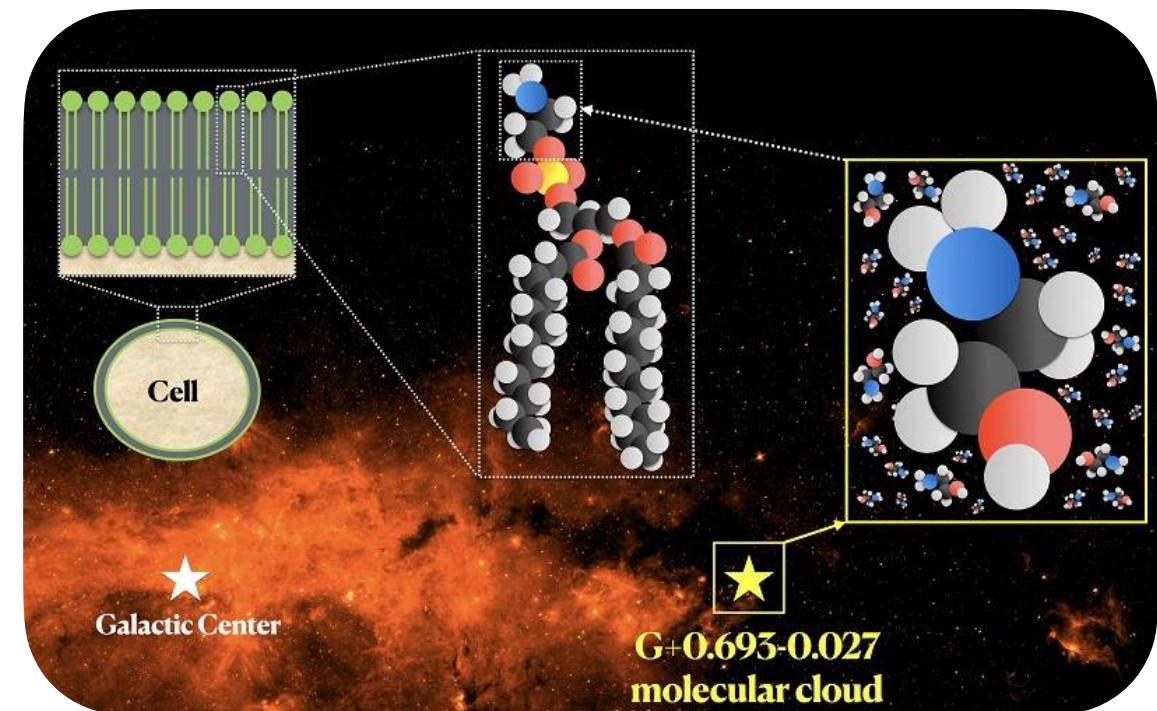


# COMPLEX ORGANIC MOLECULES



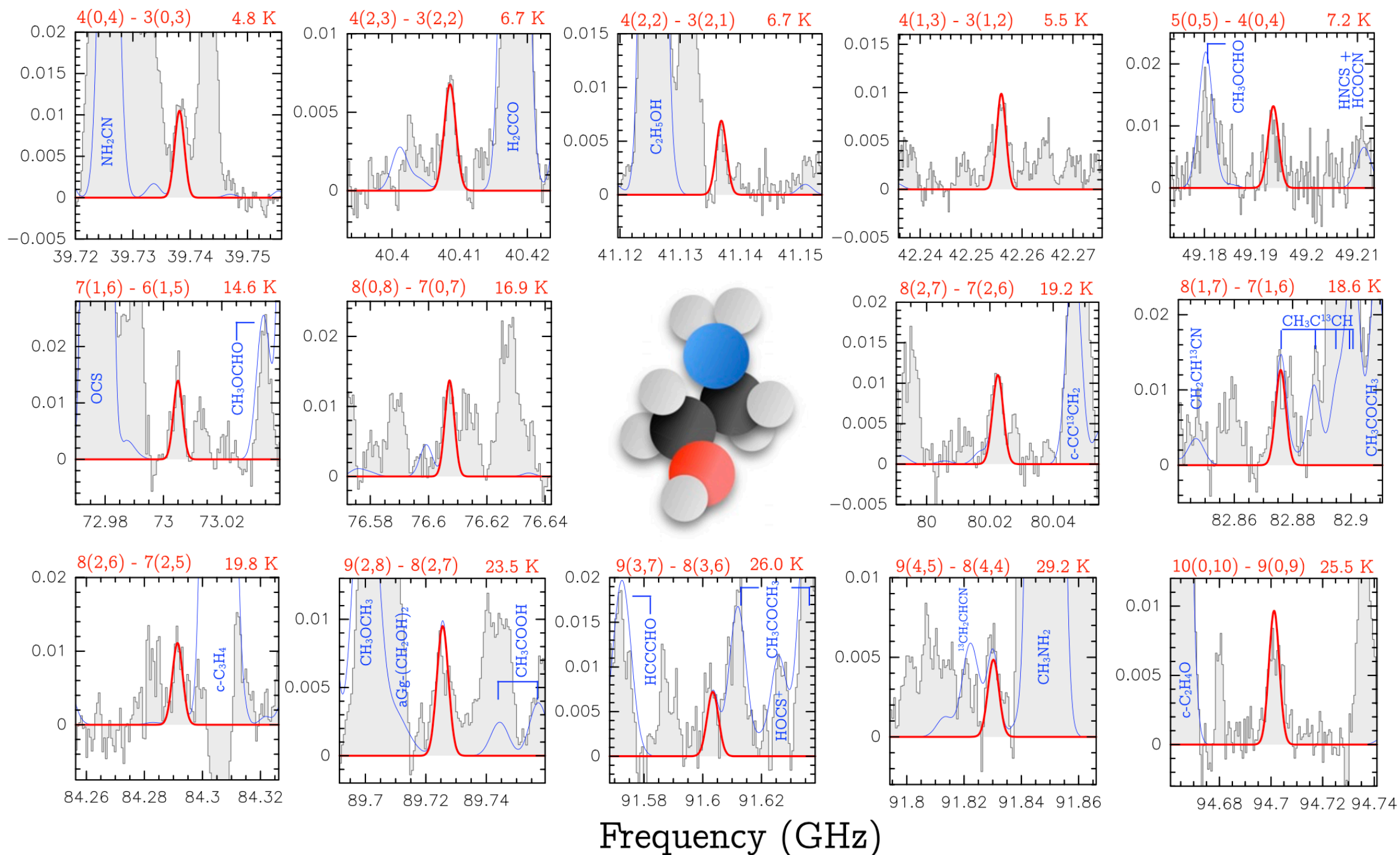
- Nitrogen (N)
- Hydrogen (H)
- Carbon (C)
- Oxygen (O)

## Ethanolamine



Relevant role in the evolution of the first cellular membranes needed for the emergence of life (from a proto-solar nebula to early Earth).

## COMPLEX ORGANIC MOLECULES (IRAM)





# LARGE MOLECULE STATISTICS

**Table 3**

List of Detected Interstellar Molecules with Eight or More Atoms, Categorized by Number of Atoms, and Vertically Ordered by Detection Year

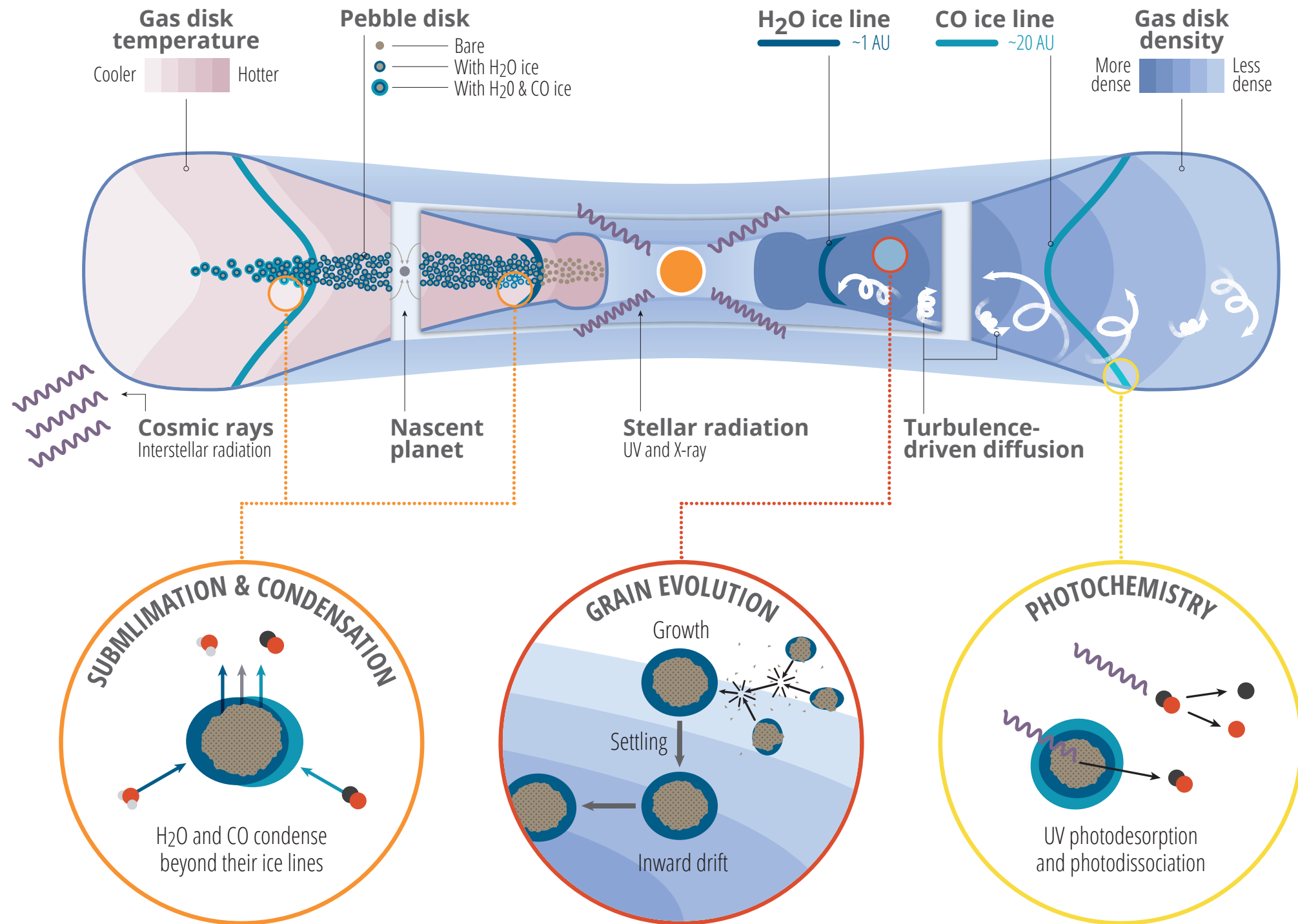
8 Atoms	9 Atoms	10 Atoms	11 Atoms	12 Atoms	13 Atoms	Fullerenes
HCOOCH <sub>3</sub>	CH <sub>3</sub> OCH <sub>3</sub>	(CH <sub>3</sub> ) <sub>2</sub> CO	HC <sub>9</sub> N	C <sub>6</sub> H <sub>6</sub>	c-C <sub>6</sub> H <sub>5</sub> CN	C <sub>60</sub>
CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> CH <sub>2</sub> OH	HO(CH <sub>2</sub> ) <sub>2</sub> OH	CH <sub>3</sub> C <sub>6</sub> H	n-C <sub>3</sub> H <sub>7</sub> CN		C <sub>60</sub> <sup>+</sup>
C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> CN	CH <sub>2</sub> CH <sub>2</sub> CHO	CH <sub>3</sub> CH <sub>2</sub> OCHO	i-C <sub>3</sub> H <sub>7</sub> CN		C <sub>70</sub>
CH <sub>3</sub> COOH	HC <sub>7</sub> N	CH <sub>3</sub> C <sub>5</sub> N	CH <sub>3</sub> COOCH <sub>3</sub>			
H <sub>2</sub> C <sub>6</sub>	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> CHCH <sub>2</sub> O				
CH <sub>2</sub> OHCHO	C <sub>8</sub> H	CH <sub>3</sub> OCH <sub>2</sub> OH				
HC <sub>6</sub> H	CH <sub>3</sub> CONH <sub>2</sub>					
CH <sub>2</sub> CHCHO	C <sub>8</sub> H <sup>-</sup>					
CH <sub>2</sub> CCHCN	CH <sub>2</sub> CHCH <sub>3</sub>					
NH <sub>2</sub> CH <sub>2</sub> CN	CH <sub>3</sub> CH <sub>2</sub> SH					
CH <sub>3</sub> CHNH	HC <sub>7</sub> O					
CH <sub>3</sub> SiH <sub>3</sub>						

**Table 9**

Total Number of Detections that Each Source Contributed to for the Molecules Listed in Section 3

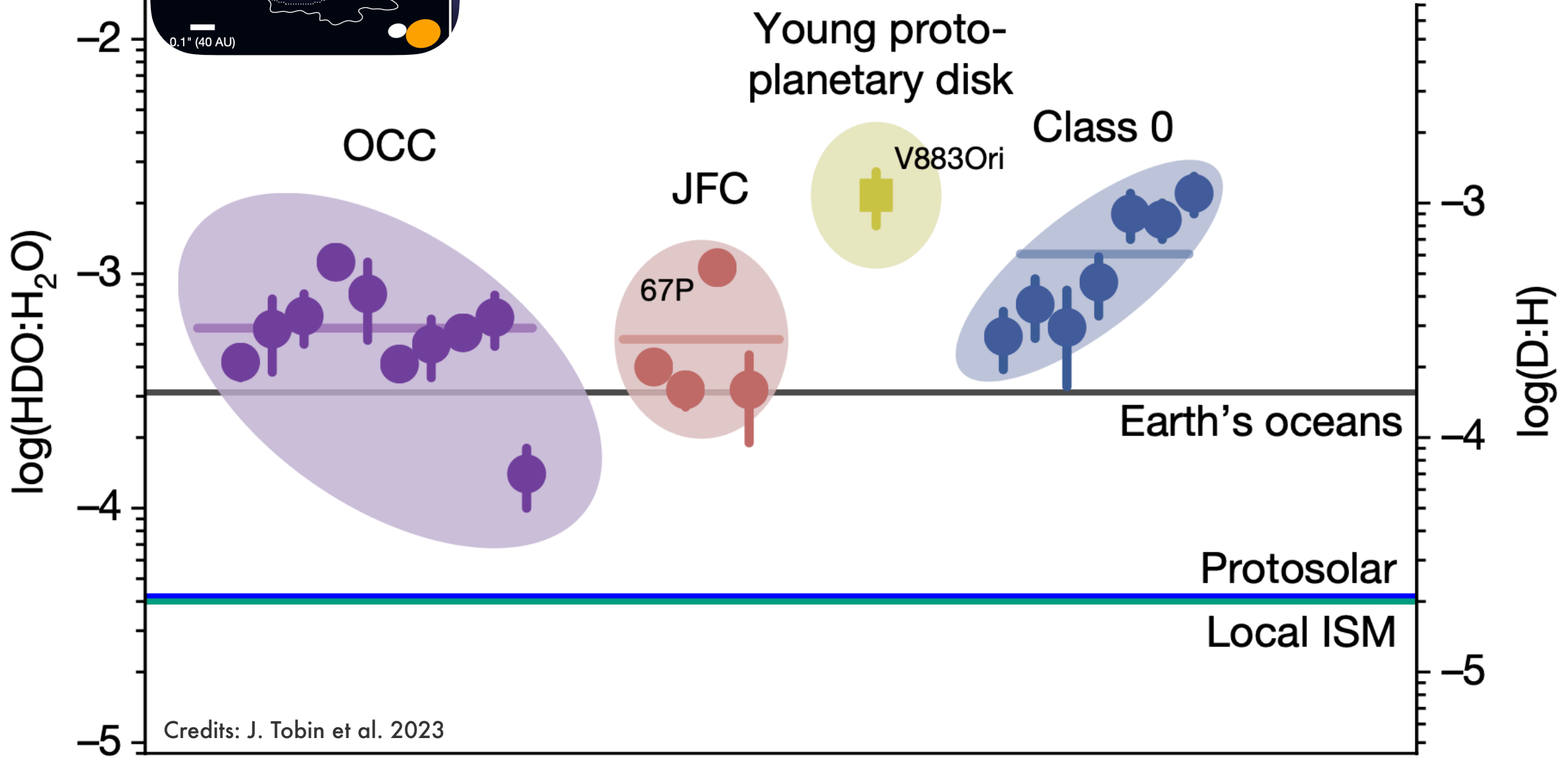
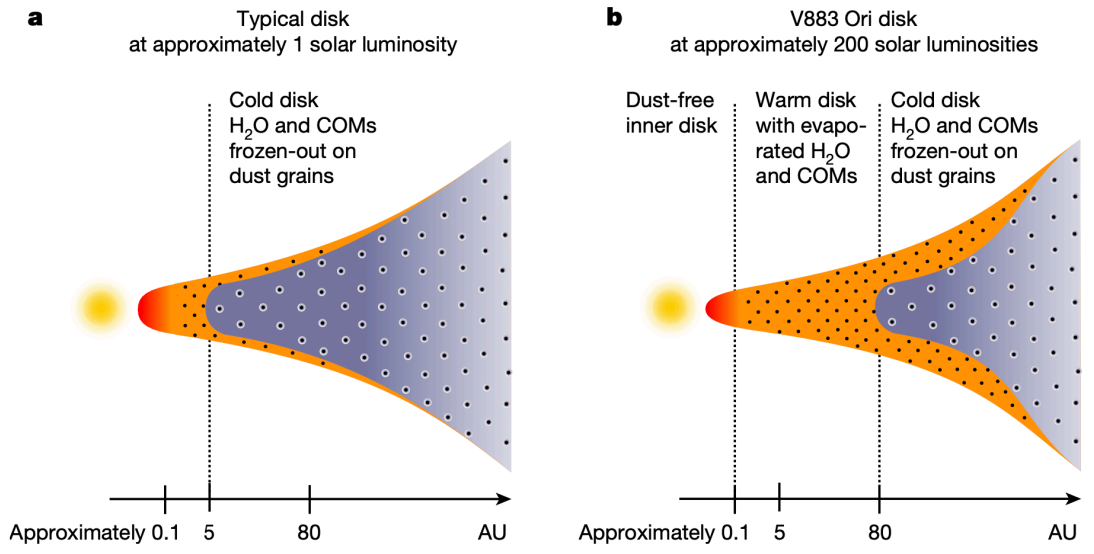
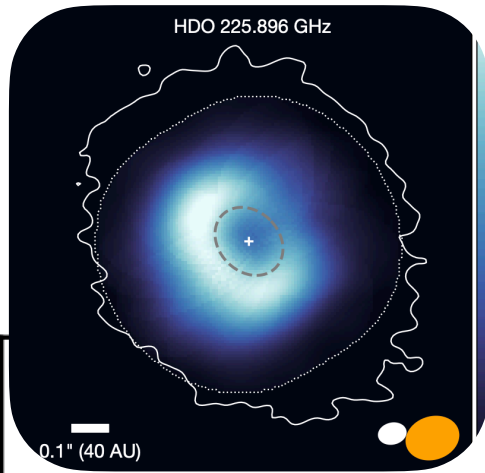
Source	#	Source	#
Sgr B2	67	NGC 7023	2
IRC+10216	51	TC 1	2
TMC-1	34	W49	2
Orion	24	CRL 2688	1
LOS Clouds	22	Crab Nebula	1
L483	8	DR 21(OH)	1
W51	8	Galactic Center	1
VY Ca Maj	5	IC 443G	1
B1-b	4	IRAS 16293	1
DR 21	4	K3-50	1
NGC 6334	4	L134	1
Sgr A	4	L1527	1
CRL 618	3	L1544	1
NGC 2264	3	L183	1
W3(OH)	3	Lupus-1A	1
rho Oph A	3	M17SW	1
Horsehead PDR	2	NGC 7027	1
NGC 2024	2	NGC 7538	1

# NEW DISCOVERIES



# NEW DISCOVERIES

in V883 Orionis the snow line is located further from the star, there is sufficient gaseous water to be detectable



Credits: J. Tobin et al. 2023





→ THE COMETARY ZOO: GASES DETECTED BY ROSETTA

THE LONG CARBON CHAINS

- Methane
- Ethane
- Propane
- Butane
- Pentane
- Hexane
- Heptane



THE AROMATIC RING COMPOUNDS

- Benzene
- Toluene
- Xylene
- Benzoic acid
- Naphtalene



THE KING OF THE ZOO  
Glycine (amino acid)



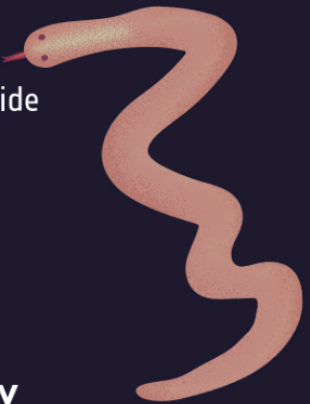
THE "MANURE SMELL" MOLECULES

- Ammonia
- Methylamine
- Ethylamine



THE "POISONOUS" MOLECULES

- Acetylene
- Hydrogen cyanide
- Acetonitrile
- Formaldehyde



THE ALCOHOLS

- Methanol
- Ethanol
- Propanol
- Butanol
- Pentanol



THE VOLATILES

- Nitrogen
- Oxygen
- Hydrogen peroxide
- Carbon monoxide
- Carbon dioxide



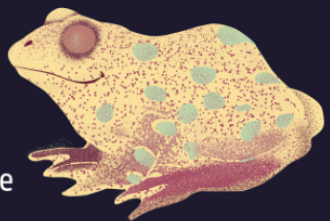
THE "SMELLY" MOLECULES

- Hydrogensulphide
- Carbonylsulphide
- Sulphur monoxide
- Sulphur dioxide
- Carbon disulphide



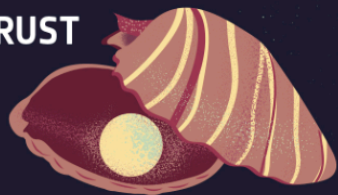
THE "SMELLY AND COLOURFUL"

- Sulphur
- Disulphur
- Trisulphur
- Tetrasulphur
- Methanethiole
- Ethanethiol
- Thioformaldehyde



THE TREASURES WITH A HARD CRUST

- Sodium
- Potassium
- Silicon
- Magnesium



THE "SALTY" BEASTS

- Hydrogen fluoride
- Hydrogen chloride
- Hydrogen bromide
- Phosphorus
- Chloromethane



THE BEAUTIFUL AND SOLITARY

- Argon
- Krypton
- Xenon



THE "EXOTIC" MOLECULES

- Formic acid
- Acetic acid
- Acetaldehyde
- Ethylenglycol
- Propylenglycol
- Butanamide



THE MOLECULE IN DISGUISE

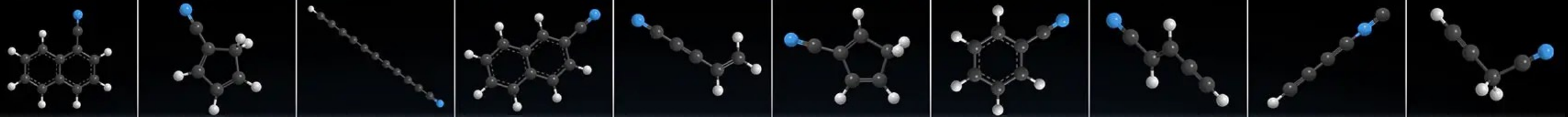
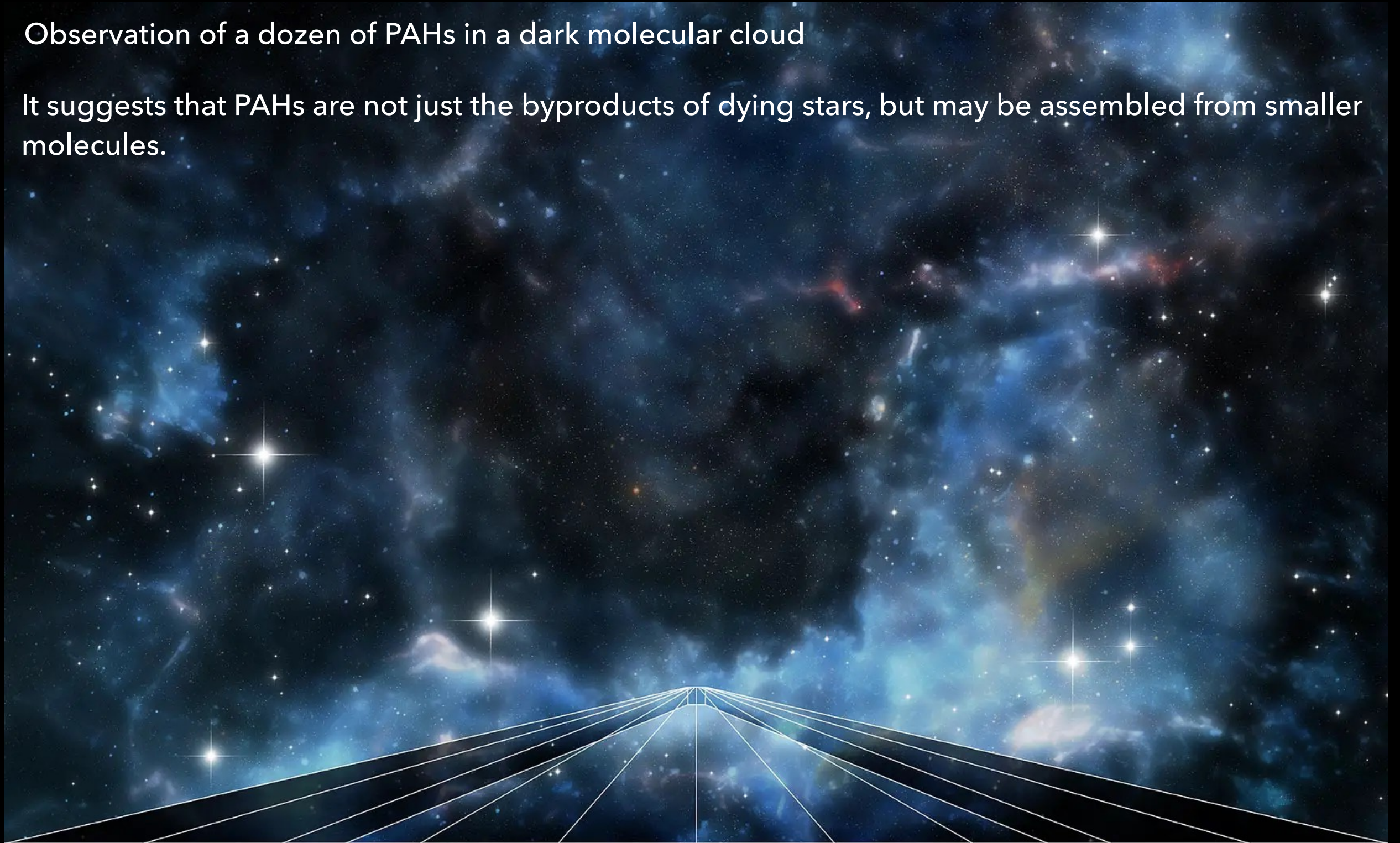
- Cyanogen





## Observation of a dozen of PAHs in a dark molecular cloud

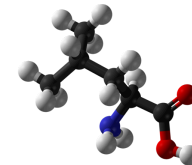
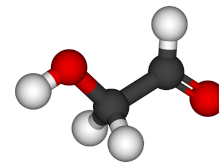
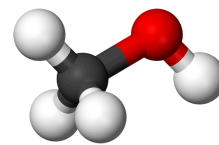
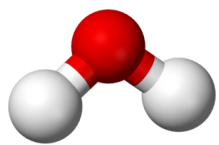
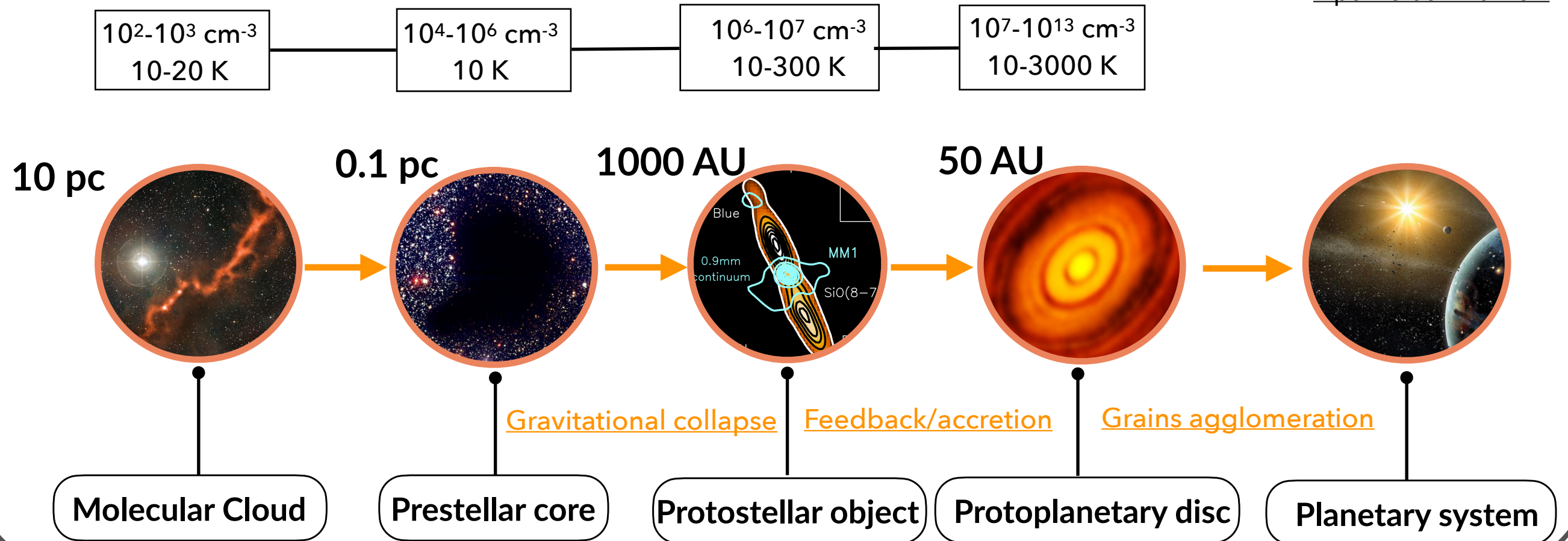
It suggests that PAHs are not just the byproducts of dying stars, but may be assembled from smaller molecules.





Star/planet formation process

1 AU =  $1.5 \times 10^{13}$  cm  
 1 pc =  $3.08 \times 10^{18}$  cm



Formation of simple molecules  
 Surface chemistry

Formation of complex molecules\*  
 Desorption due to T-increase

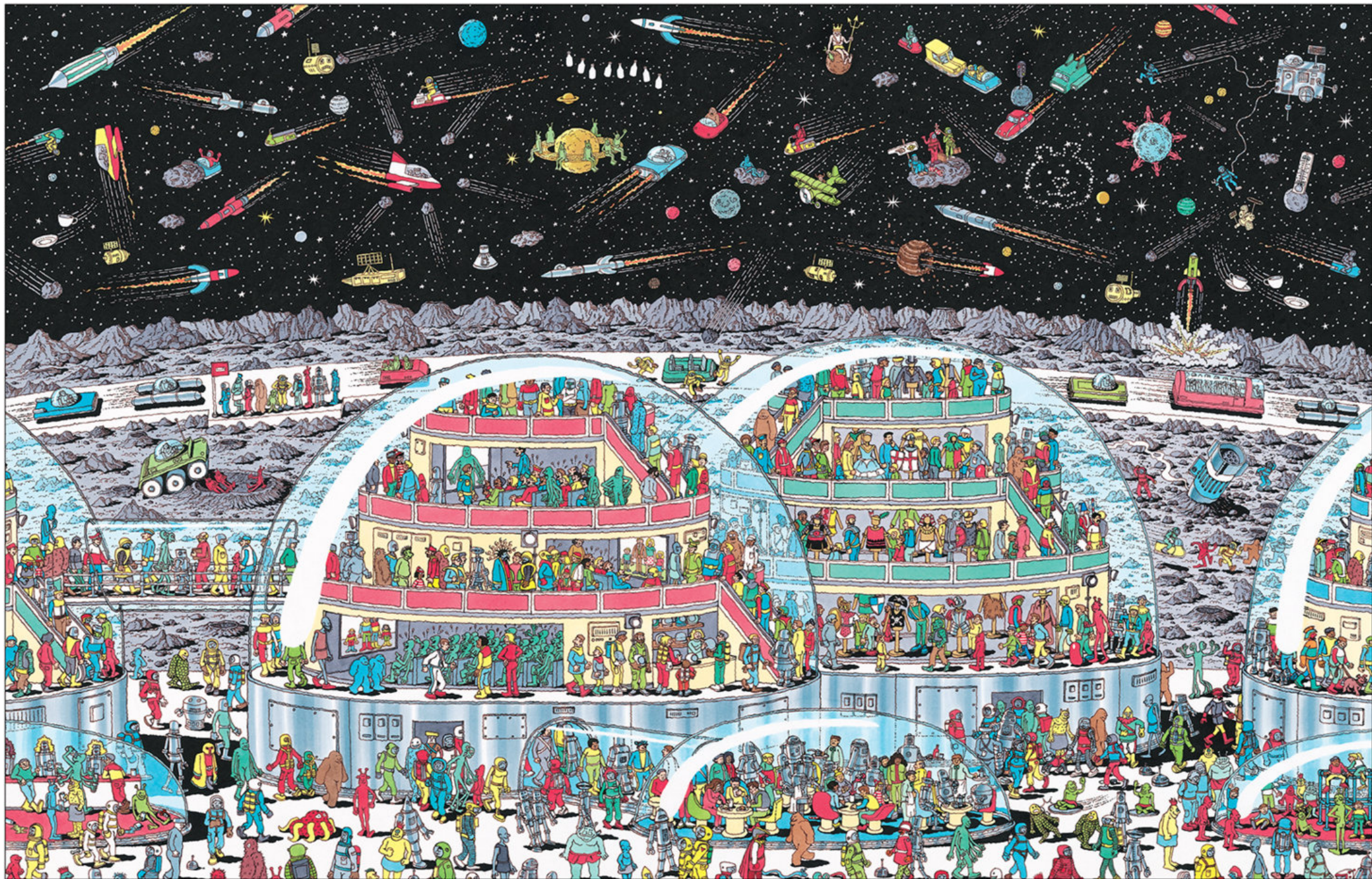
Conservation / delivery of  
 old molecules+life

Molecular Complexity

\*COMs: molecules with at least 6 atoms (must include C, Herbst & Van Dishoeck 2009)



# SEARCHING FOR MOLECULES IS NOT EASY

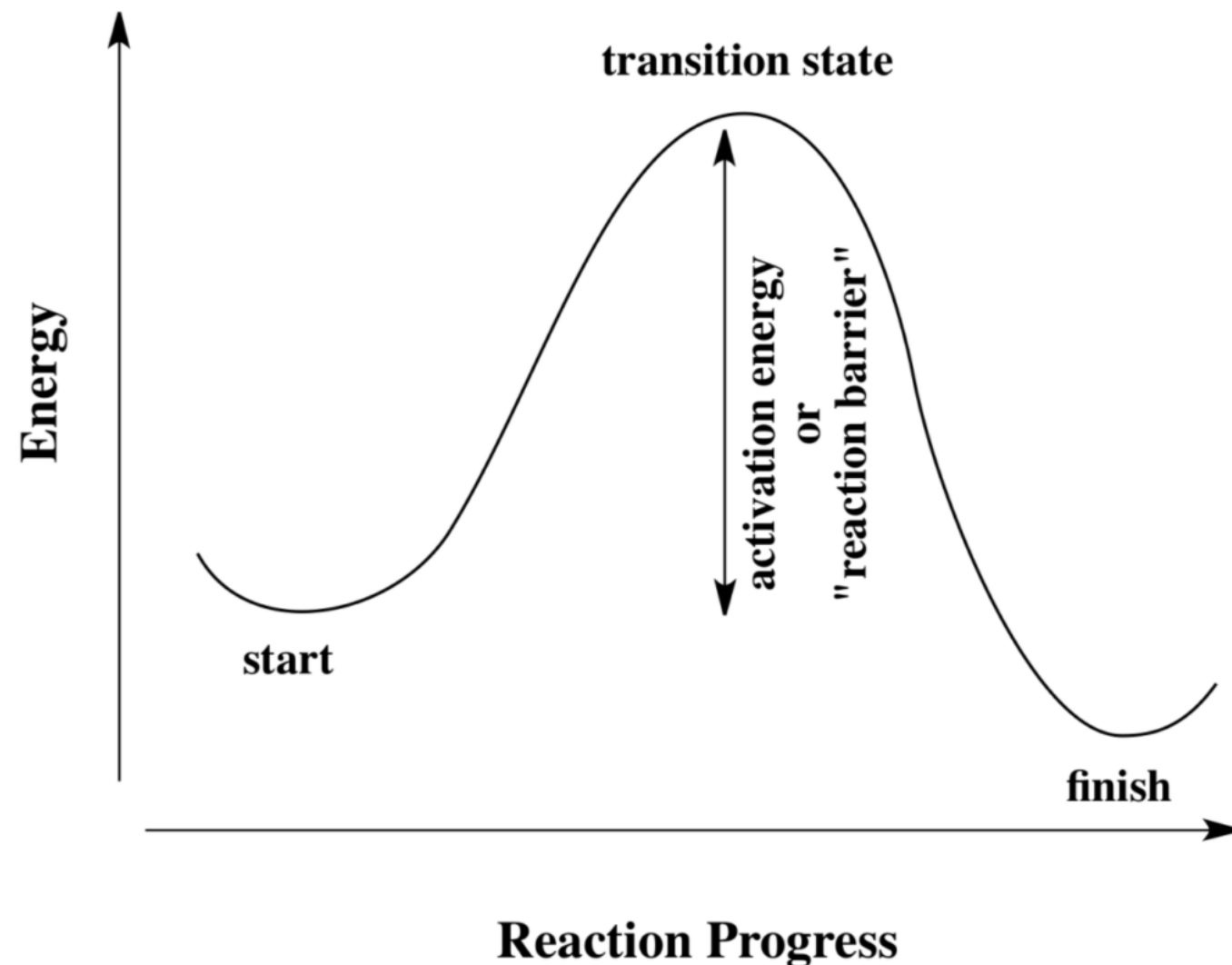


Where's Wally? In Space



# SEARCHING FOR MOLECULES IS NOT EASY

COMs and prebiotic molecules difficult to observe: need theoretical support






Kinetics / models

Provide a way to compare with observations. If the results do not match it means we miss some chemical / physical process



# SEARCHING FOR MOLECULES IS NOT EASY

How many ways I have to arrange atoms in a molecule?

-  Hydrogen (H)
-  Carbon (C)
-  Oxygen (O)



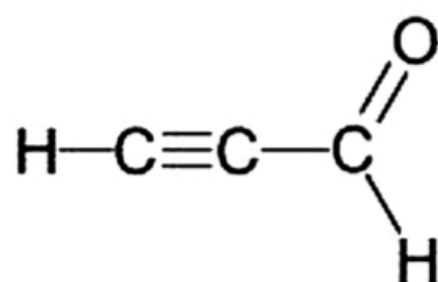
Waldo Isomer



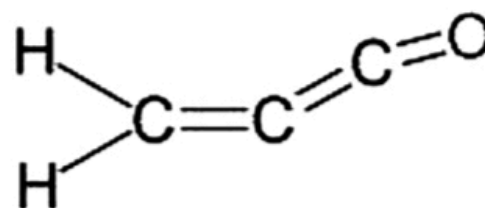
Waldo



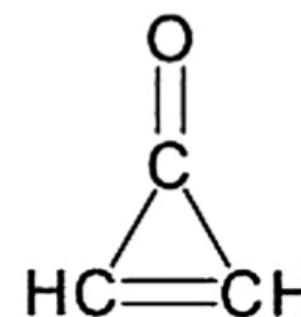
Waldo Isomer



propynal  
HCCCHO



propadienone  
CH<sub>2</sub>CCO



cyclopropenone  
*c*-H<sub>2</sub>C<sub>3</sub>O

ISOMERS

# SEARCHING FOR MOLECULES IS NOT EASY

Propadienone is the most stable isomer: is it the most abundant?



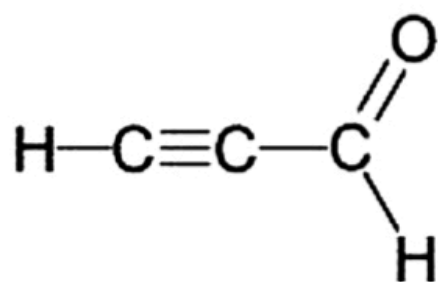
Waldo Isomer



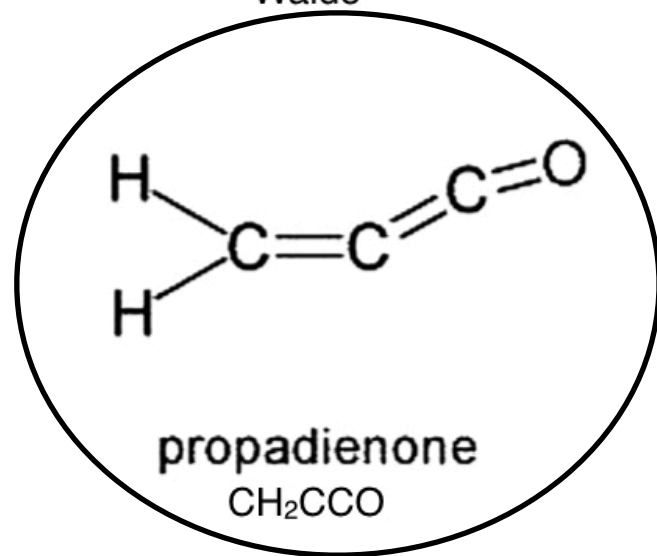
Waldo



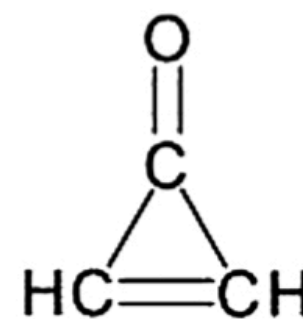
Waldo Isomer



propynal  
HCCCHO



propadienone  
CH<sub>2</sub>CCO

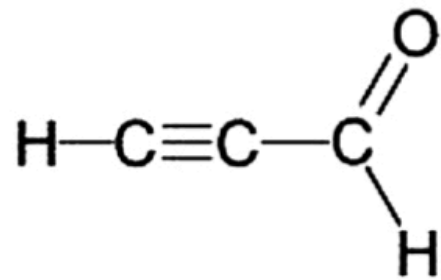


cyclopropenone  
*c*-H<sub>2</sub>C<sub>3</sub>O

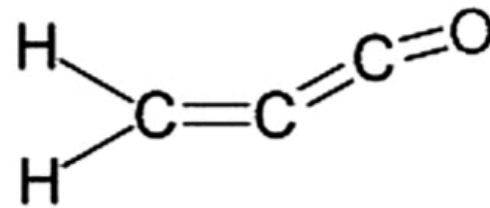


## SEARCHING FOR MOLECULES IS NOT EASY

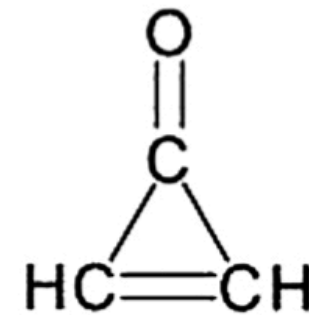
**OBSERVATIONS** question the minimum energy principle and the idea on relying on kinetics for chemical models



propynal  
HCCCHO



propadienone  
CH<sub>2</sub>CCO

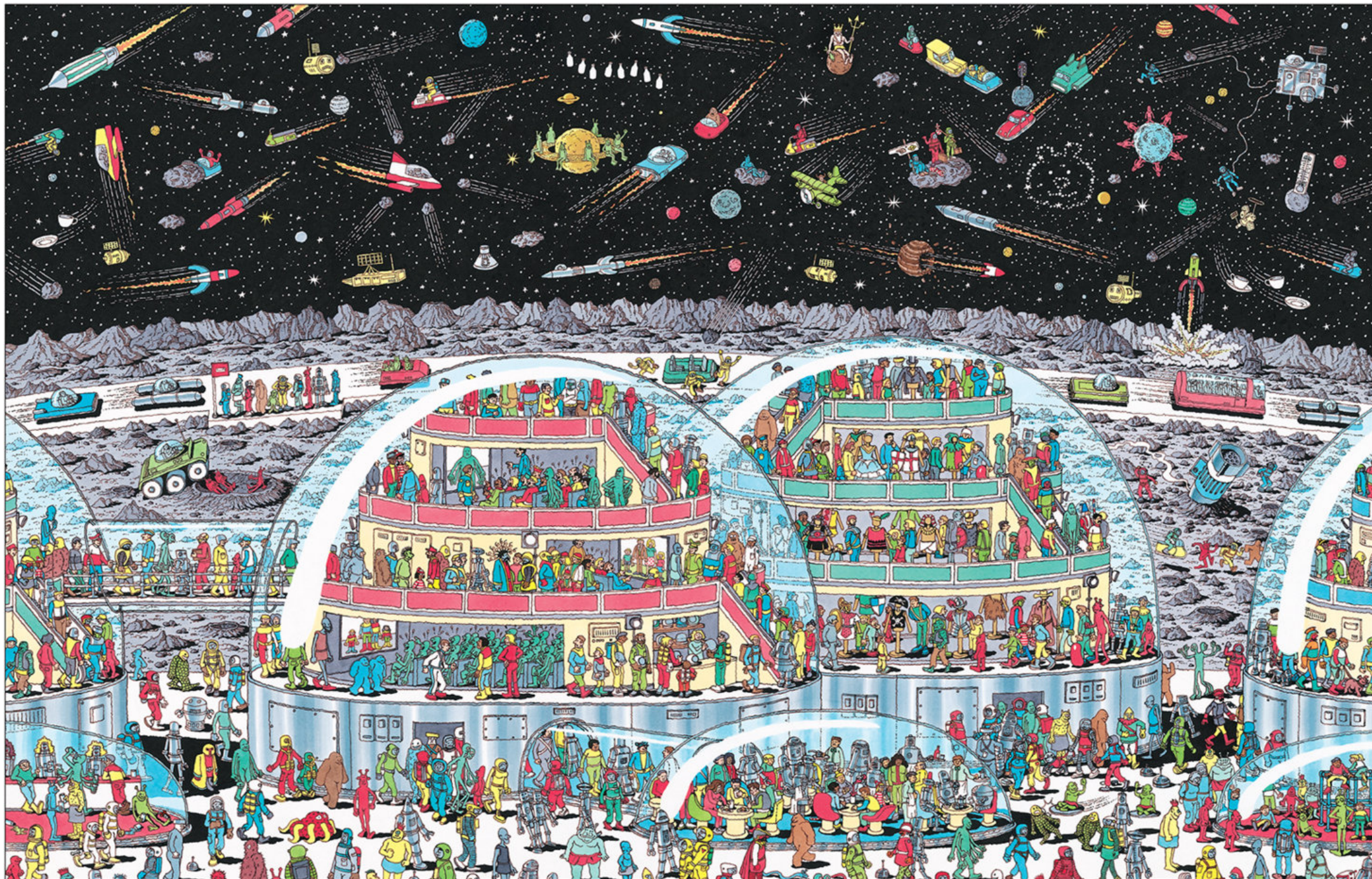


cyclopropenone  
*c*-H<sub>2</sub>C<sub>3</sub>O





# WE WILL FIND WALLY IN A FEW LECTURES



Where's Wally? In Space