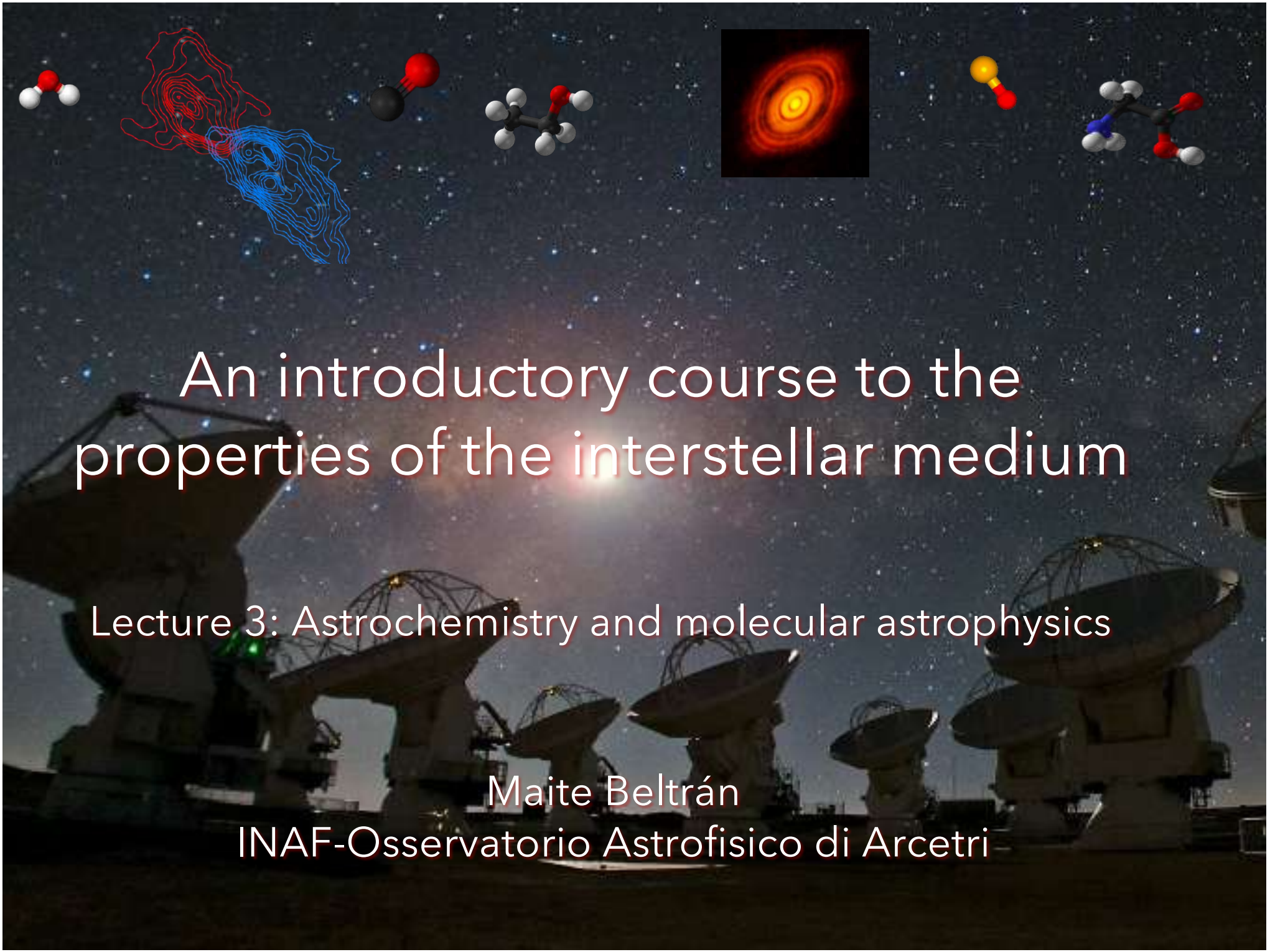
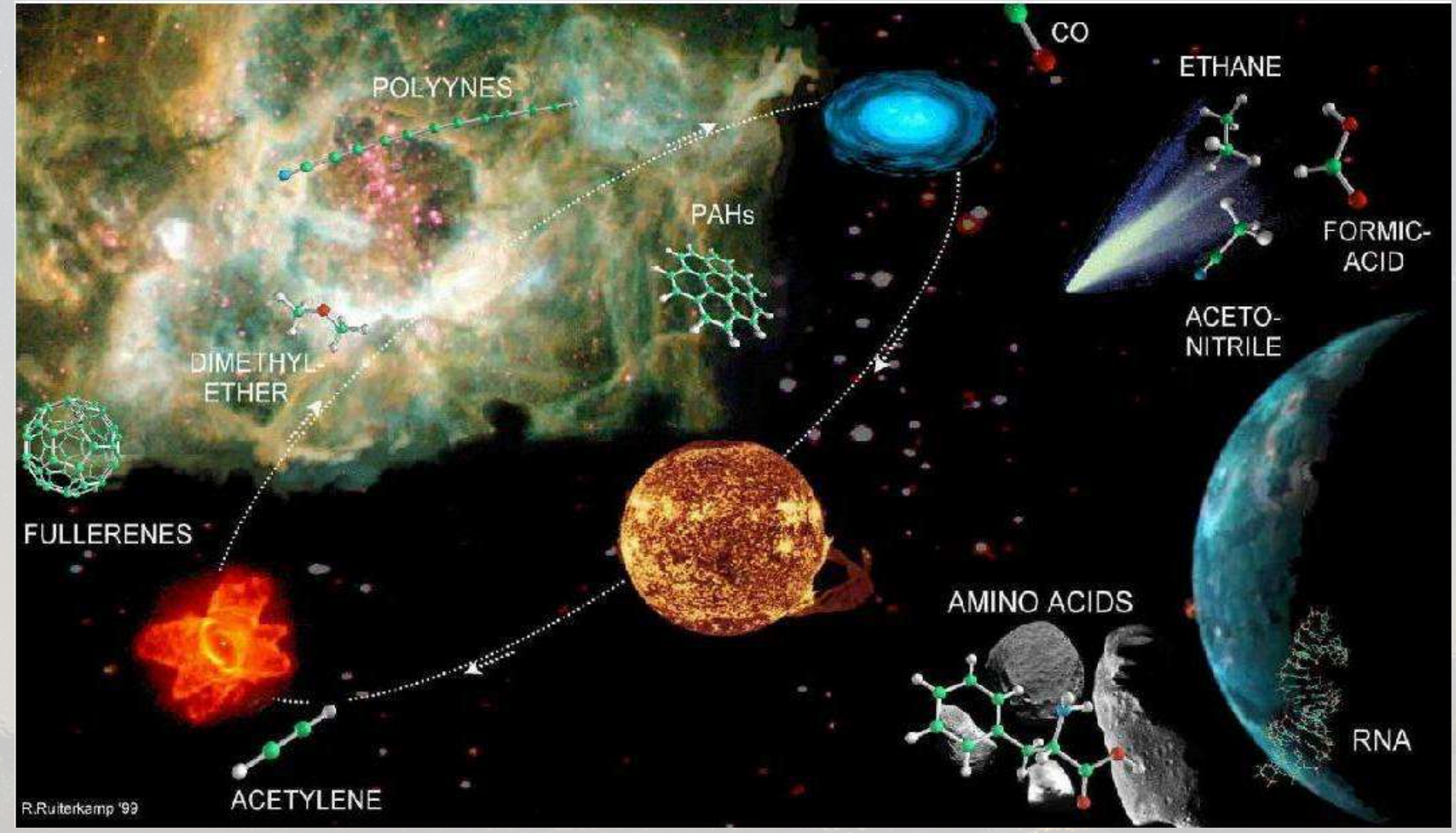


An introductory course to the properties of the interstellar medium

Lecture 3: Astrochemistry and molecular astrophysics

Maite Beltrán
INAF-Osservatorio Astrofisico di Arcetri


CO
ETHANE
POLYYNES
PAHs
FORMIC-
ACID
ACETO-
NITRILE
DIMETHYL-
ETHER
FULLERENES
AMINO ACIDS
RNA
ACETYLENE
R.Ruiterkamp '99

Summary

1. Molecules in space
2. Detection of molecules
3. Formation of molecules:
   - Surface chemistry
   - Gas-phase chemistry
4. Complex organic chemistry

References:

"Interstellar chemistry", Duley & Williams, 1984
"Introduction to astrochemistry", S. Yamamoto, 2017
"Molecular astrophysics", A. Tielens, 2021

Summary

1. Molecules in space
2. Detection of molecules
3. Formation of molecules:
   - Surface chemistry
   - Gas-phase chemistry
4. Complex organic chemistry

1. Molecules in space

Molecules in the Interstellar Medium or Circumstellar Shells (as of 02/2025)

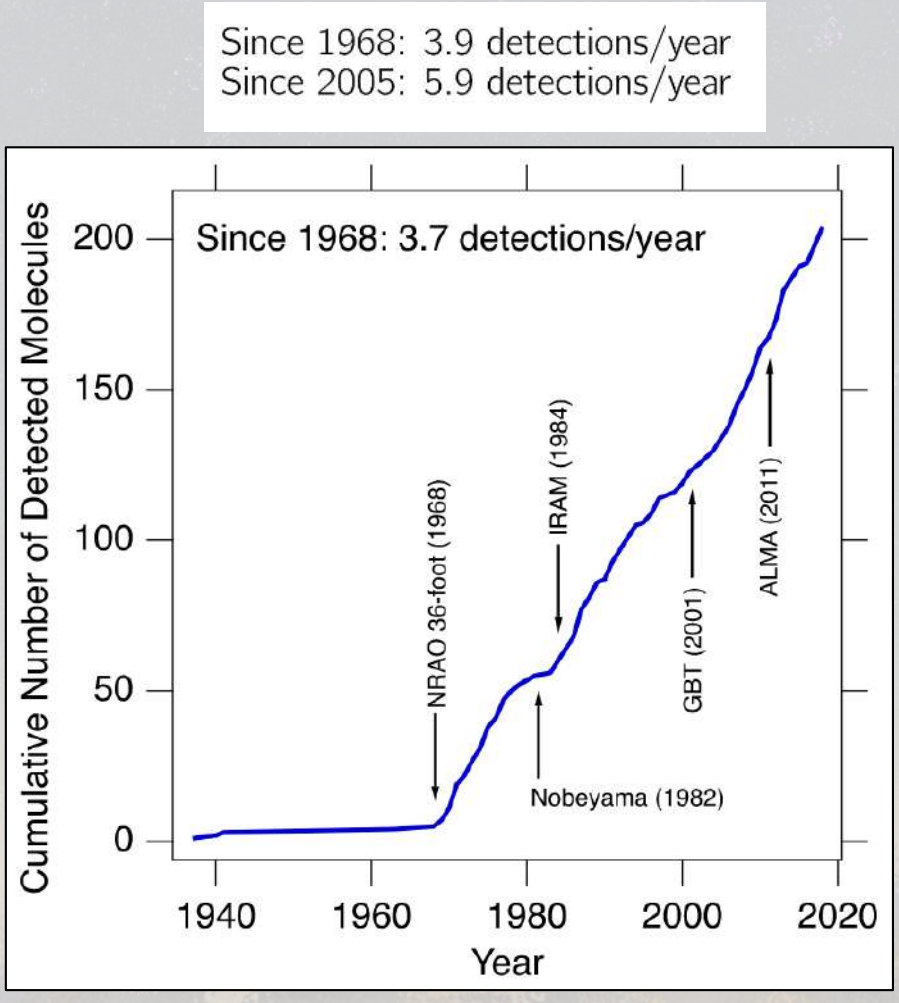
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
CH^+	C_3^*	c-C_3H	C_5^*	C_5H^-	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	c-$C_6H_6^*$	C_{60}^*
CH	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HC(O)OCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	n-C_3H_7CN	C_{70}^*
CN	C_2O	C_3N	C_4Si	$C_2H_4^*$	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$	C_2H_5OCHO	i-C_3H_7CN	C_{60}^{+*}
OH	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO	$CH_3OC(O)CH_3$	$C_2H_5OCH_3$	c-C_6H_5CN
CO	CH_2	C_3S	c-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	CH_3CHCH_2O	$CH_3C(O)CH_2OH$	1-c-C_5H_5CN	$HC_{11}N$
H_2	HCN	$C_2H_2^*$	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3OCH_2OH	c-C_5H_6	2-c-C_5H_5CN	1-$C_{10}H_7CN$
SiO	HCO	NH_3	CH_4^*	CH_3SH	c-C_2H_4O	l-HC_6H^*	$CH_3C(O)NH_2$	c-C_6H_4	$HOCH_2CH_2NH_2$	CH_3C_7N (?)	2-$C_{10}H_7CN$
CS	HCO^+	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO	C_8H^-	H_2CCCHC_3N	H_2CCCHC_4H	n-C_3H_7OH	c-C_9H_8
SO	HCS^+	$HCNH^+$	HCCNC	HCCCHO	C_6H^-	CH_2CCHCN	C_3H_6	C_2H_5NCO	$C_{10}H^-$ (2023)	i-C_3H_7OH	1-c-C_5H_5CCH
SiS	HOC^+	HNCO	HCOOH	NH_2CHO	CH_3NCO	H_2NCH_2CN	CH_3CH_2SH	$C_2H_5NH_2$ (?)	$H_2C(CH)_3CN$ (2023)	$(CH_3)_2C{=}CH_2$ (2023)	2-c-C_5H_5CCH
NS	H_2O	HNCS	H_2CNH	C_5N	HC_3O	CH_3CHNH	CH_3NHCHO	HC_7NH^+			c-$C_5H_4CCH_2$
C_2^{**}	H_2S	$HOCO^+$	H_2C_2O	l-HC_4H^+	$HOCH_2CN$	CH_3SiH_3	HC_7O	E-$CH_3CHCHCN$			2-C_9H_7CN
NO	HNC	H_2CO	H_2NCN	l-HC_4N	HCCCHNH	$H_2NC(O)NH_2$	HCCCHCHCN	Z-$CH_3CHCHCN$			C_9H_5CCH (2023)
HCl	HNO	H_2CN	HNC_3	c-H_2C_3O	HC_4NC	$HCCCH_2CN$	H_2CCHC_3N	$CH_3C(CN)CH_2$			$CH_3OCH_2CH_2OH$ (2024)
NaCl	MgCN	H_2CS	SiH_4^*	H_2CCNH	c-C_3HCCH	HC_5NH^+	$H_2CCCHCCH$	CH_2CHCH_2CN			1-$C_{12}H_7CN$ (2024)
KCl	MgNC	H_3O^+	H_2COH^+	C_5N^-	l-H_2C_5	CH_2CHCCH	HOCHCHCHO (2024)	$HOCH_2C(O)NH_2$ (2023)			5-$C_{12}H_7CN$ (2024)
AlCl	N_2H^+	c-SiC_3	C_4H^-	HNCHCN	MgC_5N	MgC_6H	HC_7N^+ (2024)	CH_3CH_2CCH (2024)			1-$C_{16}H_9CN$ (2024)
AlF	N_2O	CH_3^+	HC(O)CN	SiH_3CN	CH_2C_3N	$C_2H_3NH_2$	$CH_2(CCH)_2$ (2024				2-$C_{16}H_9CN$ (2025)
PN	NaCN	C_3N^-	HNCNH	C_5S	NC_4NH^+ (2023)	$(CHOH)_2$	$(CH_3)_2S$ (2025)				4-$C_{16}H_9CN$ (2025)
SiC	OCS	PH_3	CH_3O	MgC_4H	MgC_4N^+ (2023)	$HC_4(HC_4$					
CP	SO_2	HCNO	NH_4^+	CH_3CO^+	HC_5N^+ (2024)	C_7N^- (2023)					
NH	c-SiC_2	HOCN	H_2NCO^+	C_3H_3	HNC_5 (2024)	CH_3CHCO (2023)					
SiN	CO_2^*	HSCN	NCCNH$^+$	H_2C_3S	$CH_2(CN)_2$ (2024	MgC_6H^+ (2023)					
SO^+	NH_2	H_2O_2	CH_3Cl	HCCCHS	HCCCHCN (2025)	Z-$(CH)_2(CN)_2$ (2024					
CO^+	$H_3^{+(1)}$	C_3H^+	MgC_3N	C_5O	CH_3CHS (2025)						
HF	SiCN	HMgNC	NH_2OH	C_5H^+							
SiH?	AlNC	HCCO	HC_3O^+	HCCNCH$^+$							
FeO?	SiNC	CNCN	HC_3S^+	c-C_3C_2H							
O_2	HCP	HONO	H_2C_2S	HC_4S							
CF^+	CCP	MgC_2H	C_4S	$HMgC_3N$ (2023)							
PO	AlOH	HCCS	HC(O)SH	MgC_4H^+ (2023)							
AlO	H_2O^+	HNCN	HC(S)CN	$H_2C_3H^+$ (2023)							
OH^+	H_2Cl^+	H_2NC	HCCCO	H_2C_3N (2023)							
CN^-	KCN	$HCCS^+$	NaCCCN (2023)	$(HO)_2CO$ (2023)							
SH^+	FeCN	CH_3^+ (2023)	MgC_3N^+ (2023)	H_2CNCN (2024)							
SH	HO_2	HCNS (2024)	HC_3N^+ (2024)	NCHCCS (2024)							
HCl$^+$	TiO_2	$HOCS^+$ (2024)	HC_3S (2024)								
TiO	C_2N	HNSO (2024)	NC_3S (2024)								
ArH$^+$	Si_2C										
N_2	HS_2										
NO^+	HCS										

- ~330 have been detected in space, either in the ISM or in circumstellar shells
- 150 with 6 o more atoms
- COMs (complex organic molecules): species containing carbon and with ≥ 6 atoms

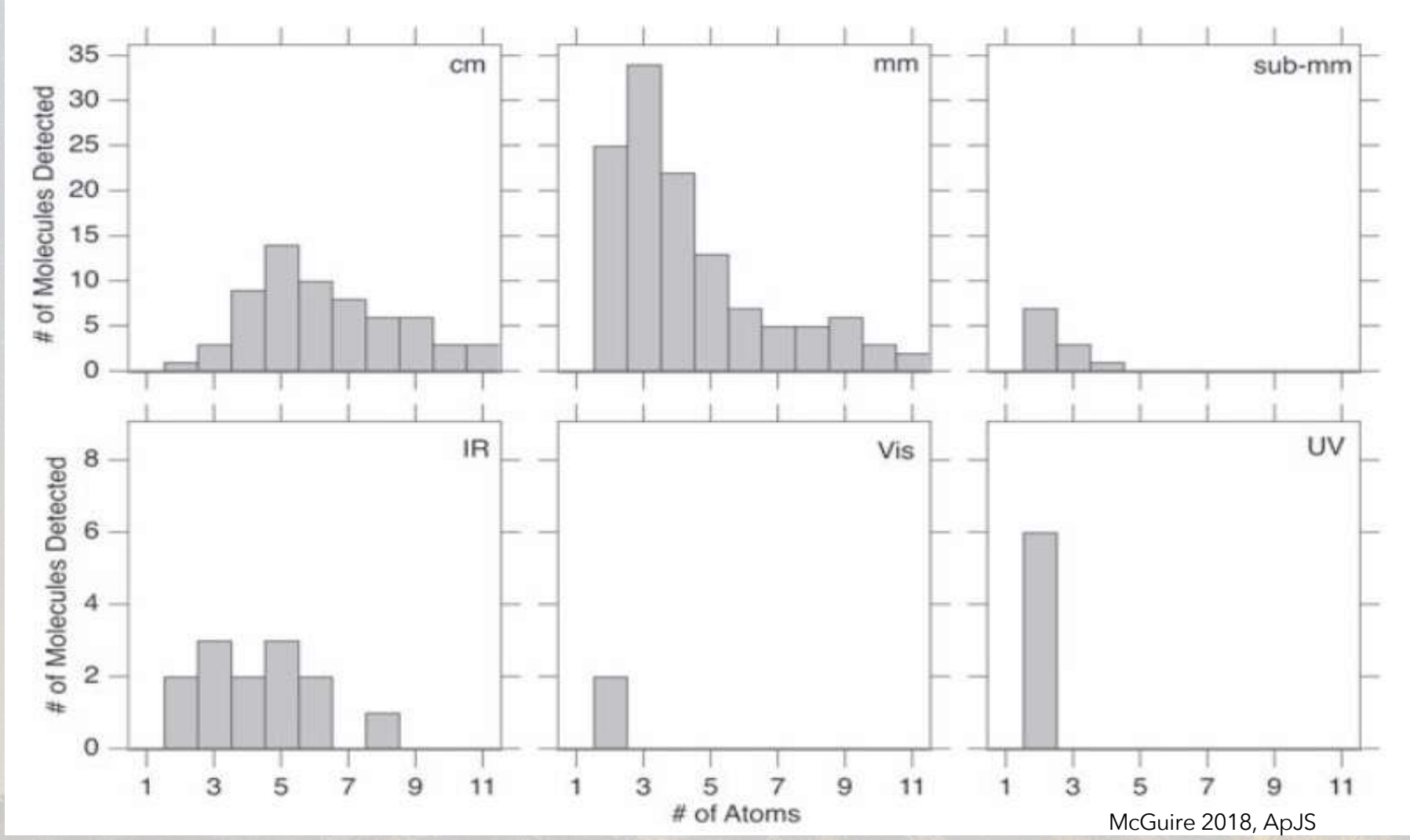
www.astro.uni-koeln.de/cdms/molecules

1. Molecules in space

- First interstellar molecular gas observations in the 1940s with the observation of absorption bands from electronic transitions in CH, CH+, and CN superimposed on the spectra of bright stars.
- In the late 1960s, cm and mm-wavelength radio observations detected emission from rotational transitions of OH (hydroxyl), CO (carbon monoxide), NH_3 (ammonia), and H_2CO (formaldehyde), discovered in 1969.
- CH_3OH is the first COM detected in space in 1970.



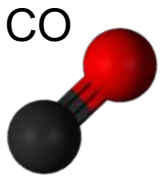
1. Molecules in space



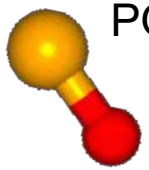
McGuire 2018, ApJS

The mm band is crucial for new detections!

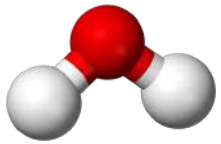
1. Molecules in space



carbon monoxide

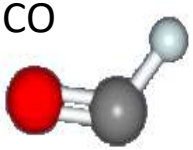


phosphorus monoxide

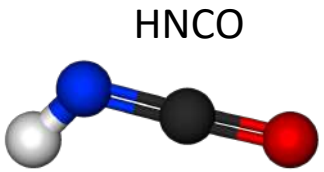


water

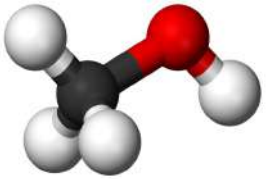
hydrogen cyanide



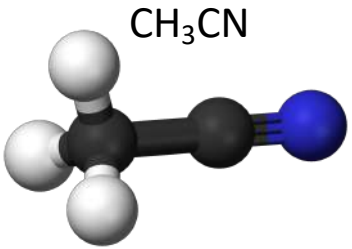
formyl radical



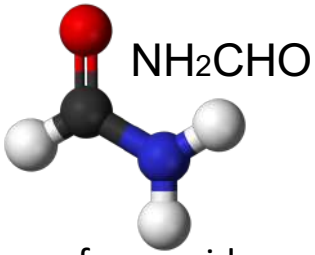
isocyanic acid



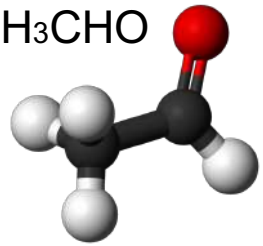
methanol



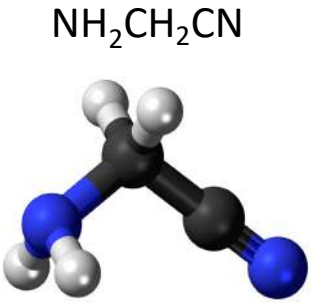
methyl cyanide



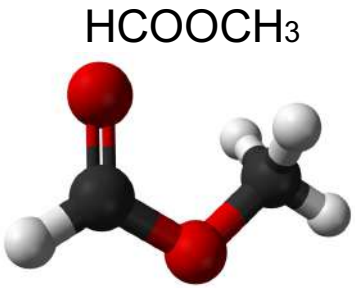
formamide



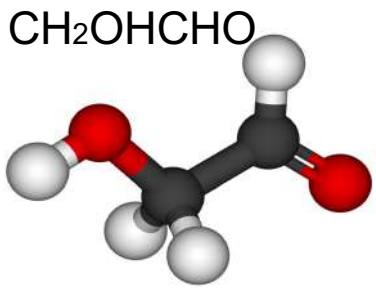
acetaldehyde



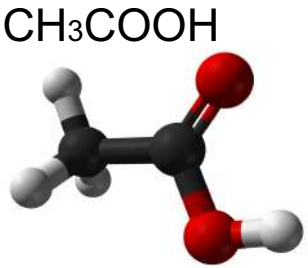
acetonitrile



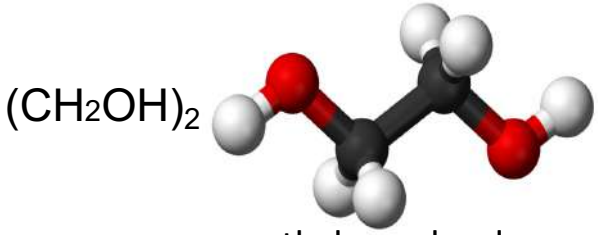
methyl formate



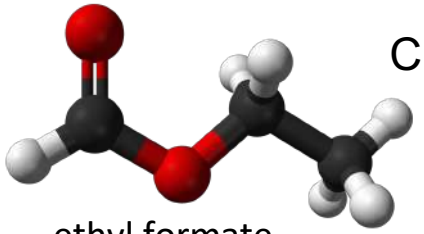
glycolaldehyde



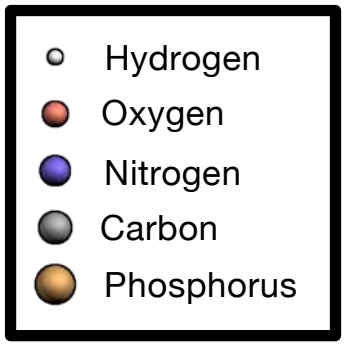
acetic acid



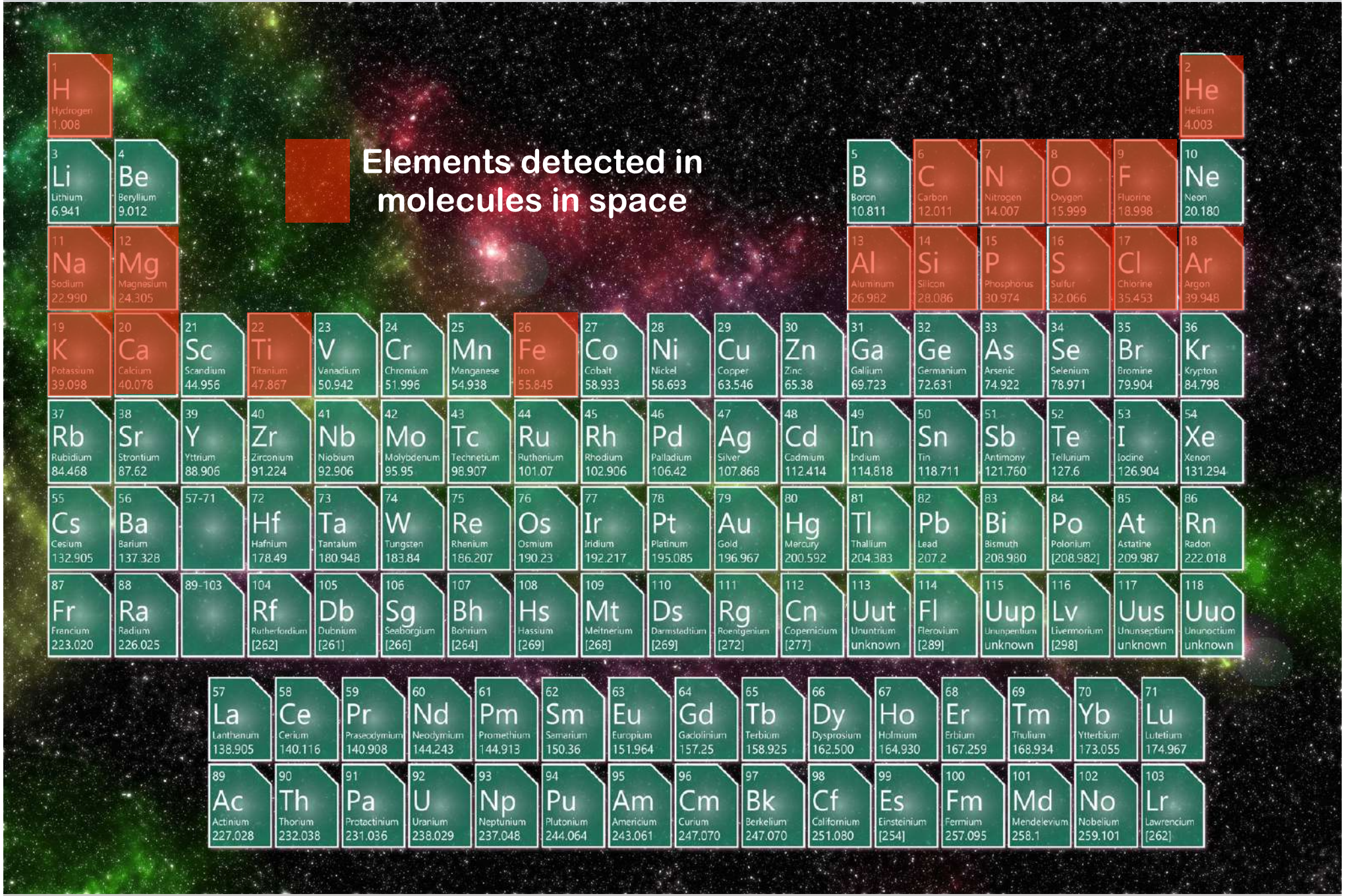
ethylene glycol



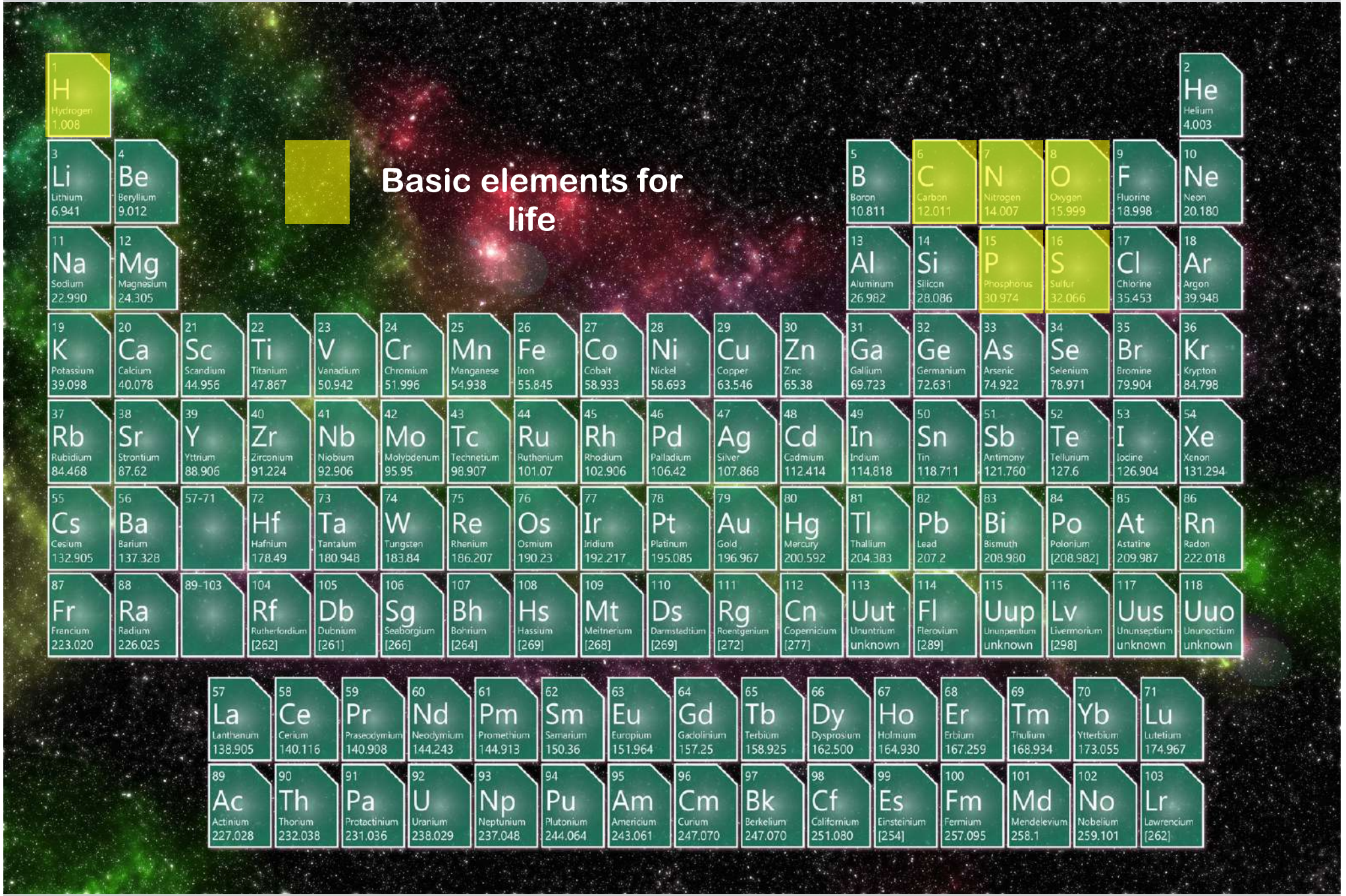
ethyl formate



1. Molecules in space



1. Molecules in space



Summary

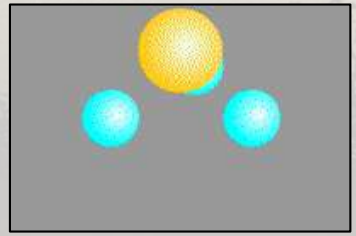
1. Molecules in space
2. Detection of molecules
3. Formation of molecules:
   - Surface chemistry
   - Gas-phase chemistry
4. Complex organic chemistry

4. Detection of molecules

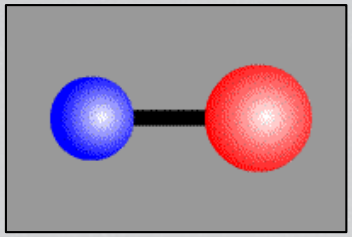
- The atoms in molecules can vibrate or rotate around an axis, emitting or absorbing pulses of energy known as photons at a certain frequency (radio, sub-millimeter, IR)

- We study interstellar molecules by observing the spectral lines they emit due to their **rotational** and **vibrational** transitions.

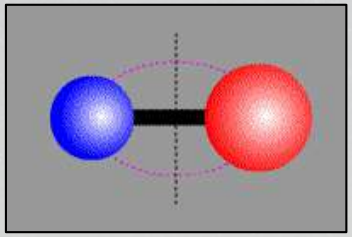
- A three-dimensional molecule such as NH_3 emits electromagnetic radiation by reversing its configuration (inverse transition).



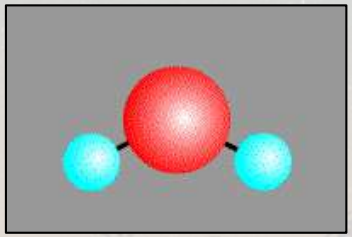
vibrational transition on CO

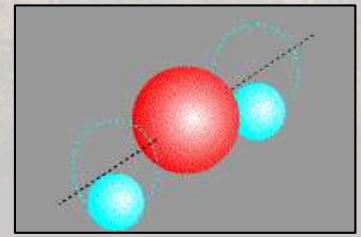


rotational transition o CO



rotational transition of H_2O

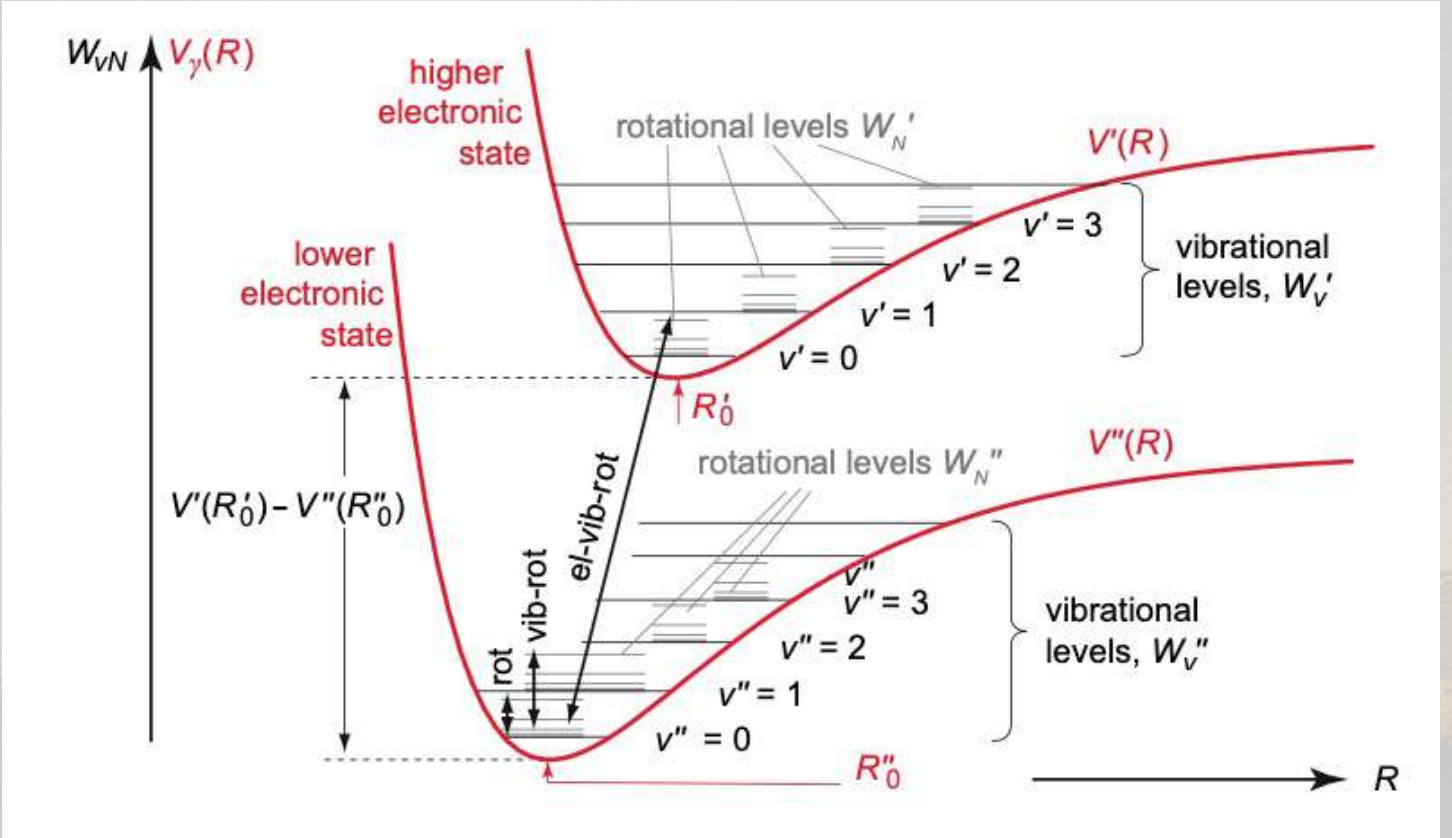




2. Detection of molecules

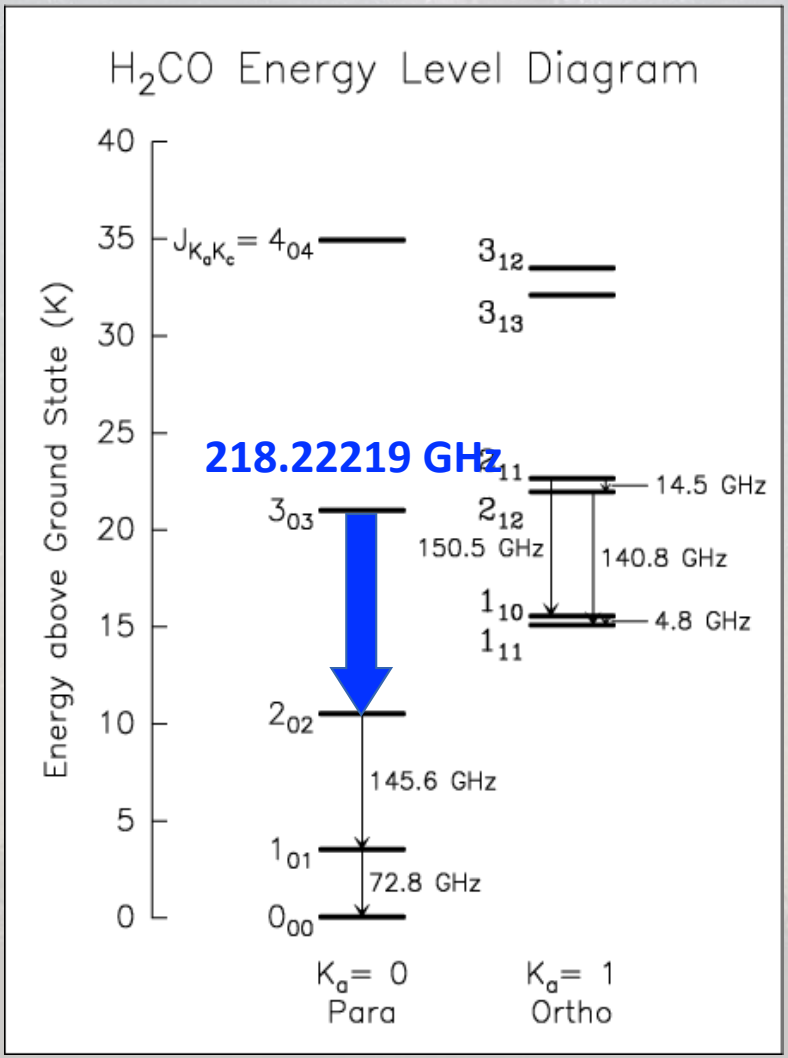
- A molecule can also present electronic transitions (which involve a change in the distribution of the electron cloud). This type of transition also occurs in atoms, while the other two are exclusive to molecules.

$$E_{tot} = E_{\text{rot}} + E_{\text{vib}} + E_{\text{el}}$$

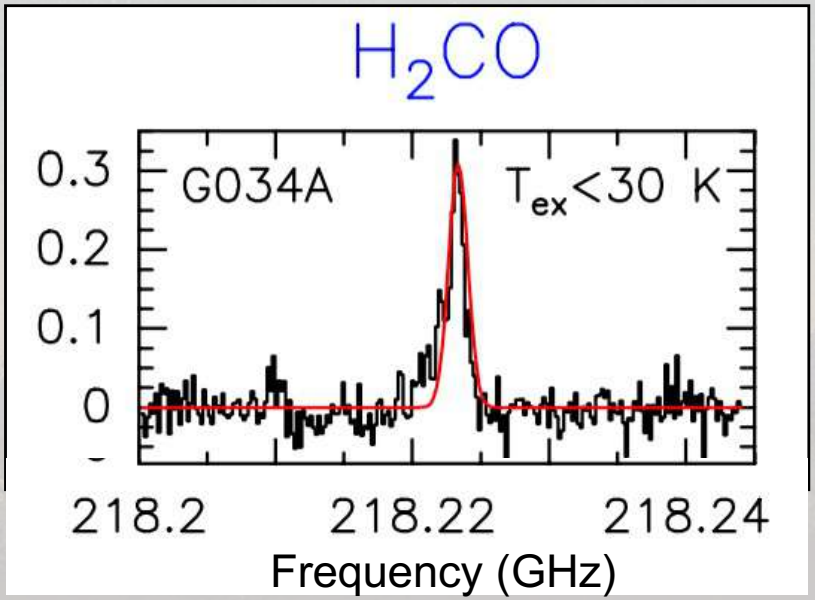


2. Detection of molecules

When the vibrational or rotational state of a certain molecule changes discretely, obeying quantum dynamics, they emit or absorb photons at a certain frequency, producing molecular lines.

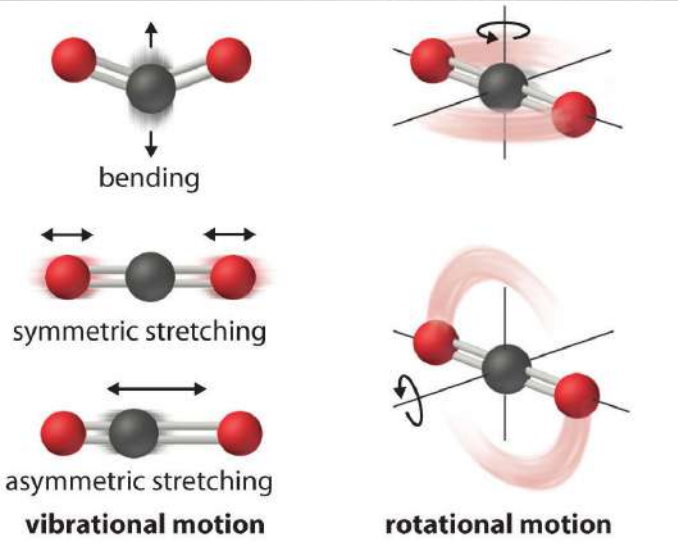


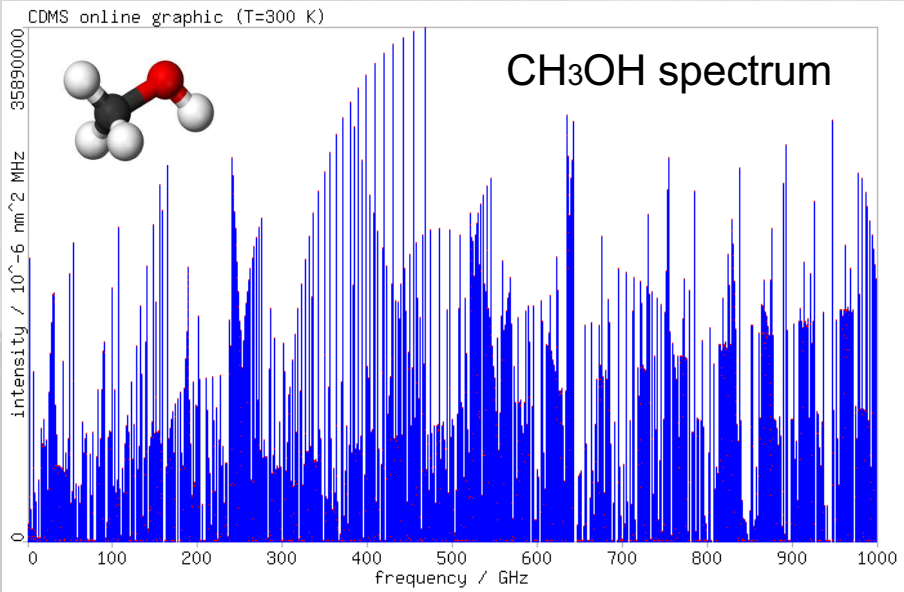
$$E = h\nu = \frac{hc}{\lambda}$$

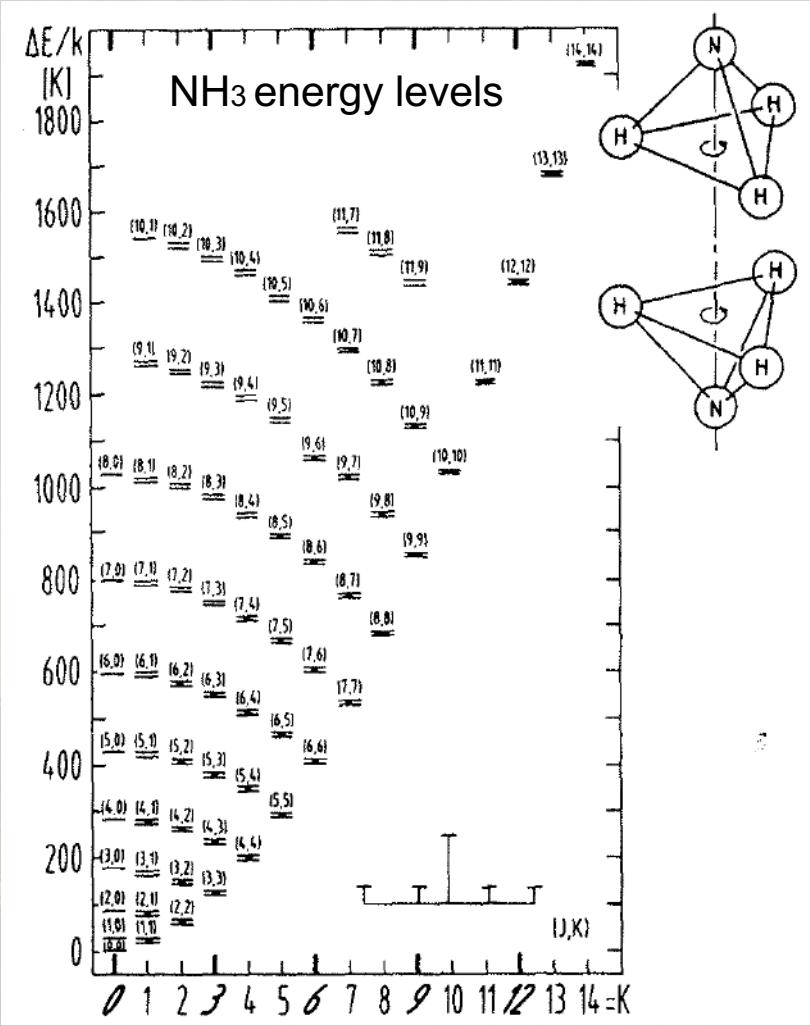


2. Detection of molecules

Each molecule produces a unique spectrum.







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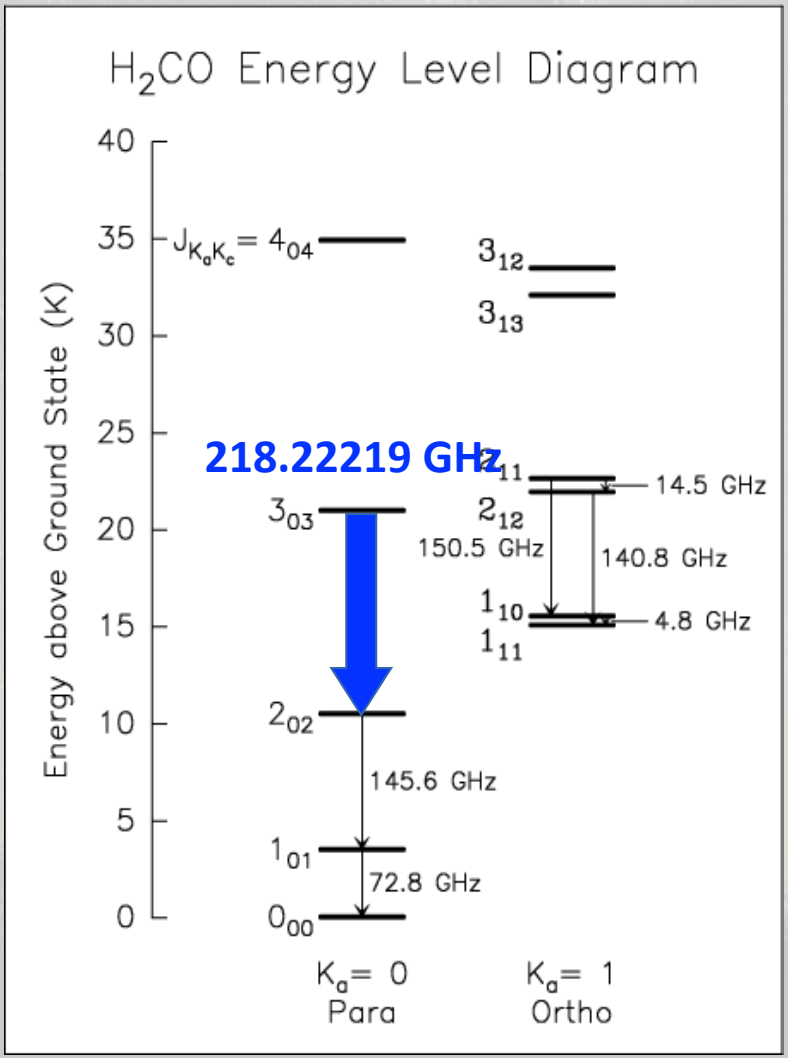


$$E = h\nu = \frac{hc}{\lambda}$$

Linear molecule

$E_J = hB_{rot}\, J(J+1)$

$E_{J+1} - E_J = h\nu = h(2J+1)B_{rot}$

where B_{rot} is the rotational constant of a molecule that represents the spacing between its rotational energy levels and it's a function of the moment of inertia I: $B_{rot} = \frac{h}{8\pi^2 I}$

B_{rot} ~ 1 – 200 GHz
→ ν ~ 1 – 200 GHz (for J=0)
→ ν ~ 3 – 600 GHz (for J=1)

Summary

1. Molecules in space
2. Detection of molecules
3. Formation of molecules:
   - Surface chemistry
   - Gas-phase chemistry
4. Complex organic chemistry

3. Formation of molecules

The most elementary chemical reaction is the radiative association of A and B to form the AB molecule, which will have an internal energy:

$$A + B \rightarrow AB^*$$

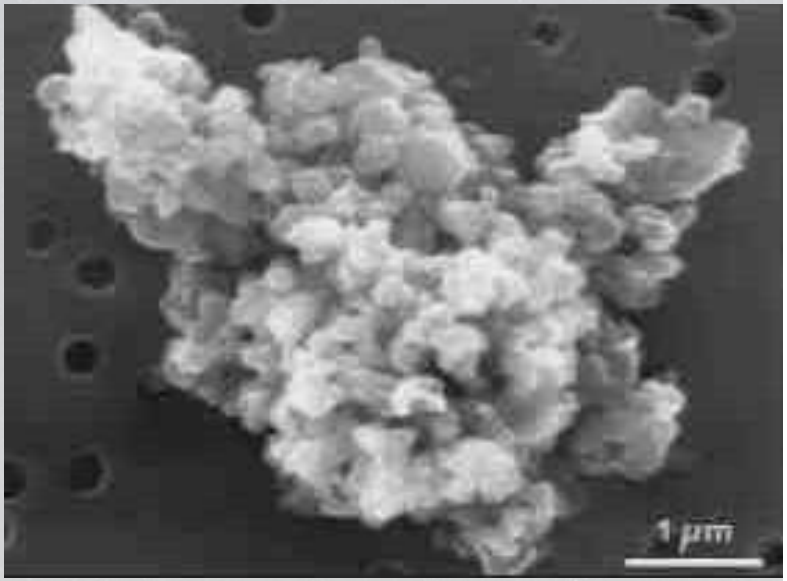
The AB* molecule MUST lose the excess energy to stay attached during impact. In the Earth's atmosphere, where the density is ~ 10^{19} cm^{-3}, the molecule loses its energy via three-body reactions:

$$AB^* + M \rightarrow AB + M^*$$

But this is not an efficient process in molecular ISM, where the number of particles per cm^{-3} goes from a few hundred to 10^7 cm^{-3}.

The dust grains, thanks to their enormous thermal capacity, can easily absorb excess energy

3a. Surface chemistry



Processes:

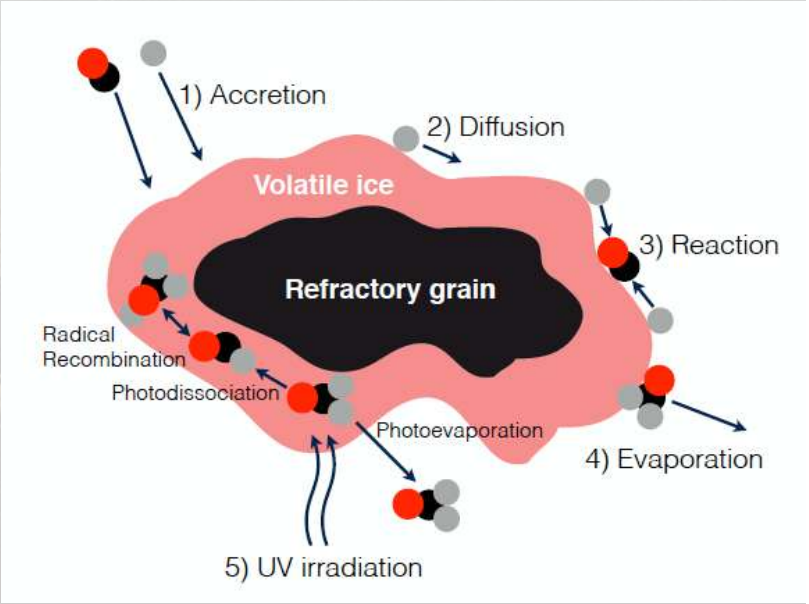
1. ACCRETION: A particle that impacts a grain can be adsorbed (i.e., remains on the surface) if the temperature is low enough. Two possible accretion processes:

   a) Physisorption: (physical adsorption) van der Waals forces (distance-dependent interactions between atoms or molecules) (0.01-0.2 eV)

   b) Chemisorption: (chemical adsorption) chemical bond (1eV)

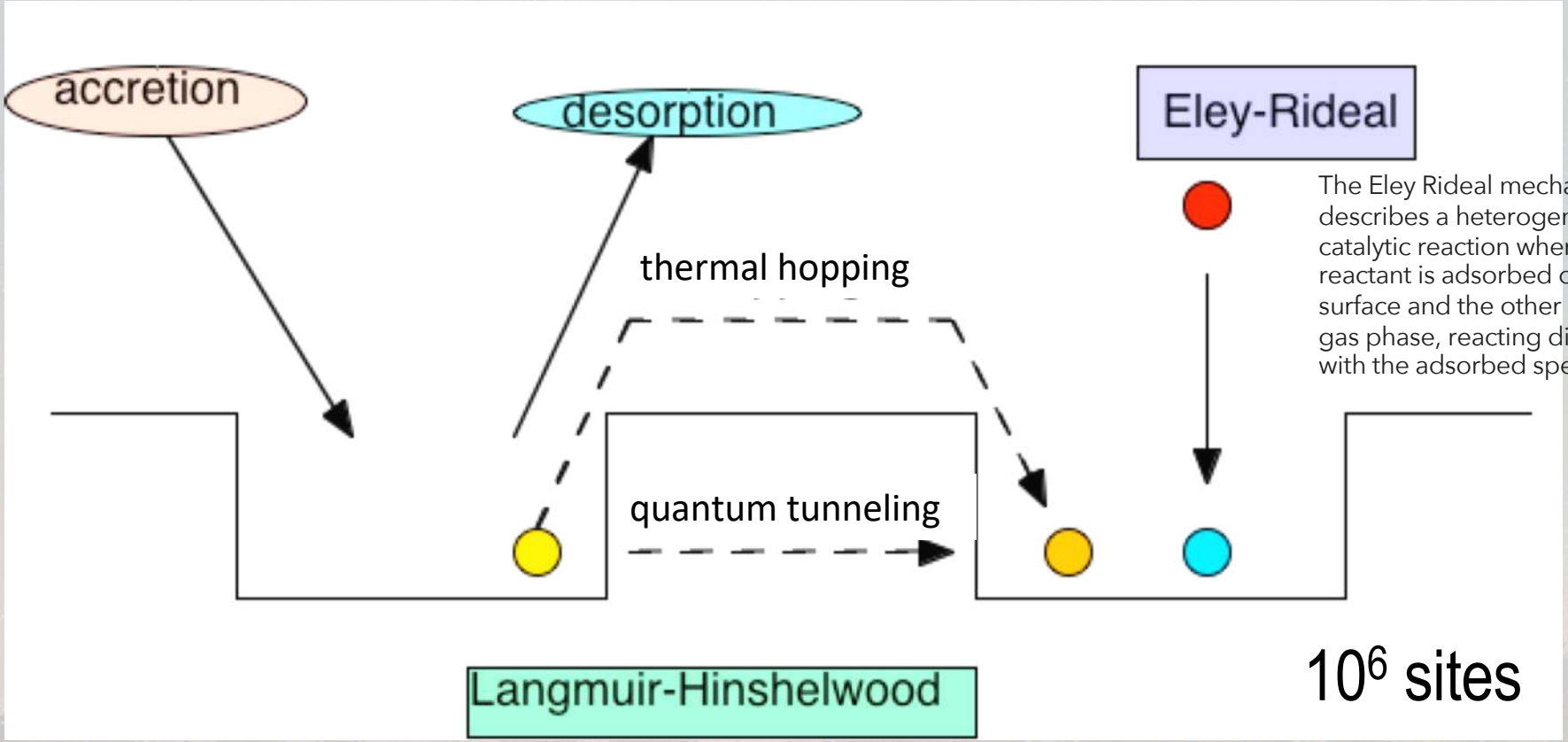
2. SURFACE DIFFUSION: if the particle is NOT tied via a chemical bond, it can move on the surface (t << 1s), and react with others: diffusion through

   a) thermal hoping
   b) quantum tunneling



3a. Surface chemistry

The "sites" where there is the greatest likelihood of forming molecules are the holes of gravitational potential (hollows) on the surface of the grain



The Eley Rideal mechanism describes a heterogeneous catalytic reaction where one reactant is adsorbed on a surface and the other is in the gas phase, reacting directly with the adsorbed species

The Langmuir-Hinshelwood mechanism involves the adsorption of two different gas molecules on separate active sites of a catalyst, followed by a reaction between the two adsorbed species.

Review recommended: Caselli et al. 2005

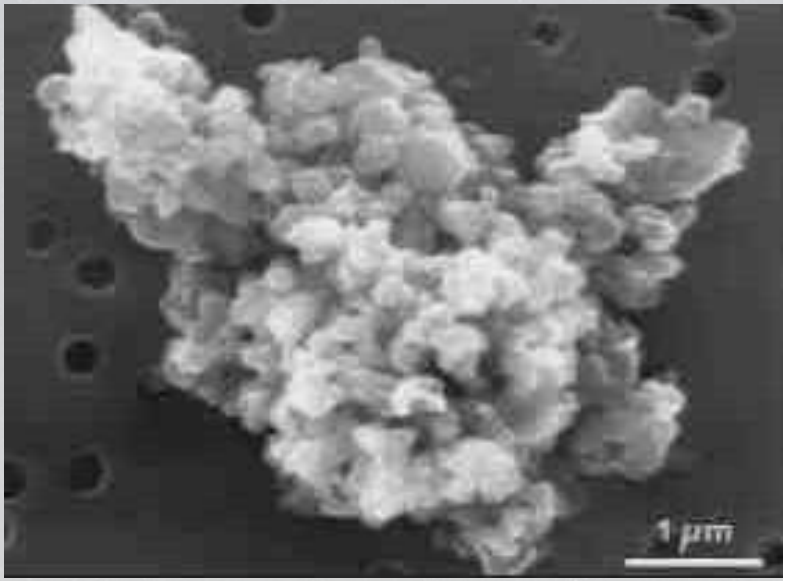
3a. Surface chemistry

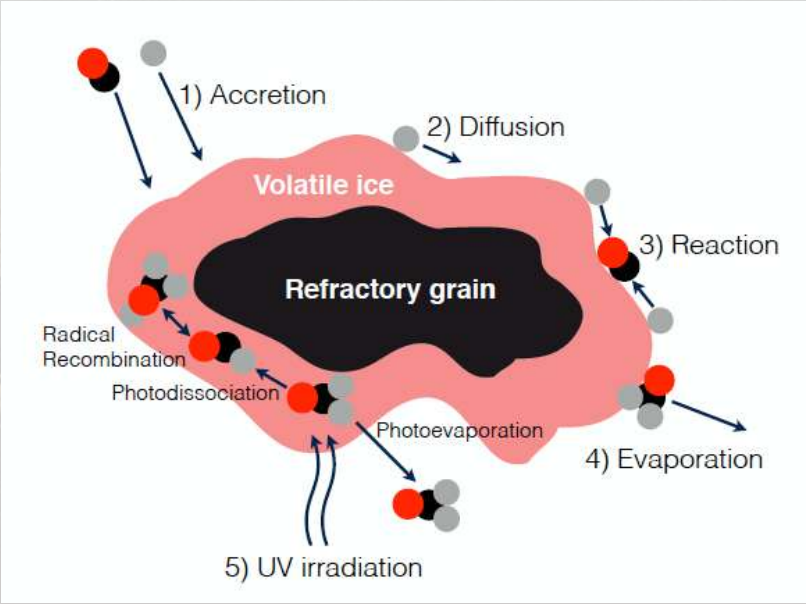
Processes:

3. REACTION through Langmuir-Hinshelwood or Eley Rideal mechanisms

4. DESORPTION:
   a) Thermal desorption
   b) Grain heating by CRs
   c) Chemical desorption: for exothermic reactions if the temperature rises above the evaporation threshold

5. UV Photolysis: photodesorption or photodissociation (if UV radiation breaks the molecule)





3a. Surface chemistry

These molecules are formed this way:

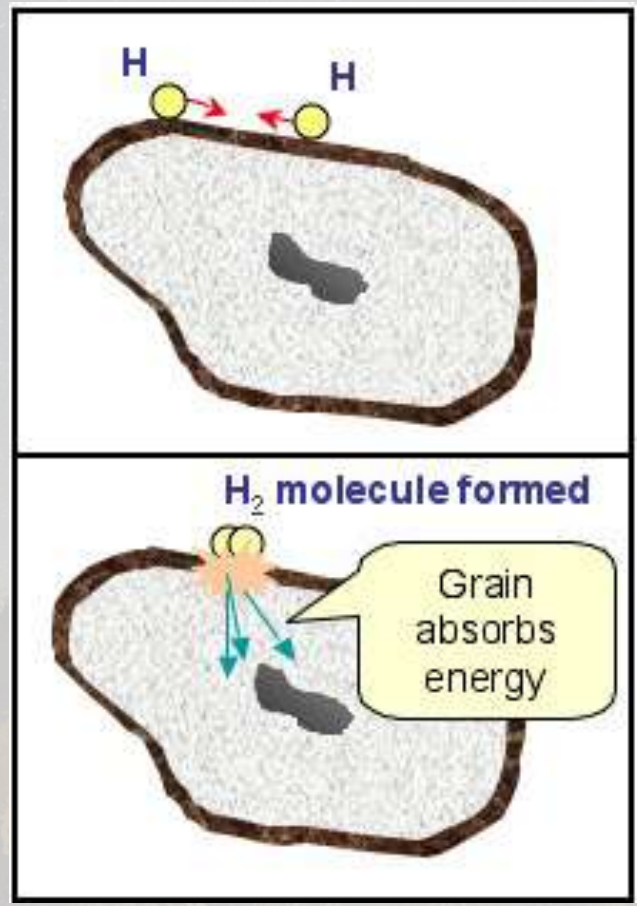
$$H \rightarrow H_2$$

$$O \rightarrow OH \rightarrow H_2O$$

$$C \rightarrow CH \rightarrow CH_2 \rightarrow CH_3 \rightarrow CH_4$$

$$N \rightarrow NH \rightarrow NH_2 \rightarrow NH_3$$

$$CO \rightarrow HCO \rightarrow H_2CO \rightarrow H_3CO \rightarrow CH_3OH$$



Watson & Salpeter (1972); Allen & Robinson (1977); Pickes & Williams (1977); d'Hendecourt et al. (1985); Hasegawa et al. (1992); Caselli et al. (1993)

3a. Gas-phase chemistry

a) neutral-neutral (atom-molecule): $A + BC \rightarrow AB + C$

b) ion-neutral: $A^+ + BC \rightarrow AB^+ + C$

c) Radiative association: $(A + B \rightarrow AB + h\nu)$

d) Dissociative recombination: $(AB^+ + e \rightarrow A + B)$

e) Charge exchange (special case of b): $A + B^+ \rightarrow A^+ + B$

f) Reactions with negative ions (special case of b)

Recommended reading "Interstellar chemistry" (Duley & Williams)

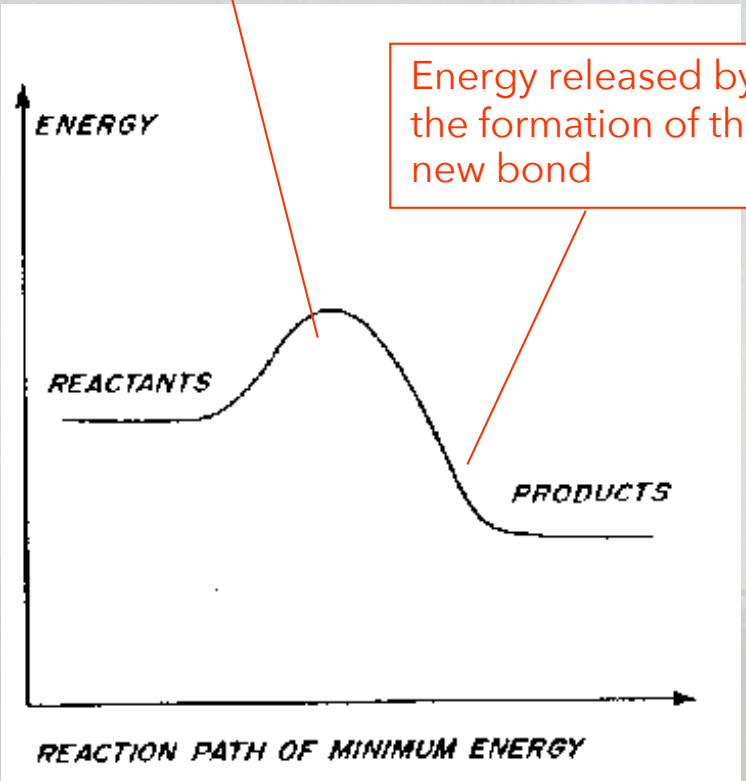
3b. Gas-phase chemistry

a. neutral-neutral: activation barrier

A + BC → AB + C

Minimum energy to break the reagent bond

Energy released by the formation of the new bond



E ~ 0.1-1 eV for exothermic reactions

$k_b T$ < 0.01 eV in molecular clouds

ONLY EXOTHERMIC REACTIONS CAN OCCUR IN THE MOLECULAR CLOUDS

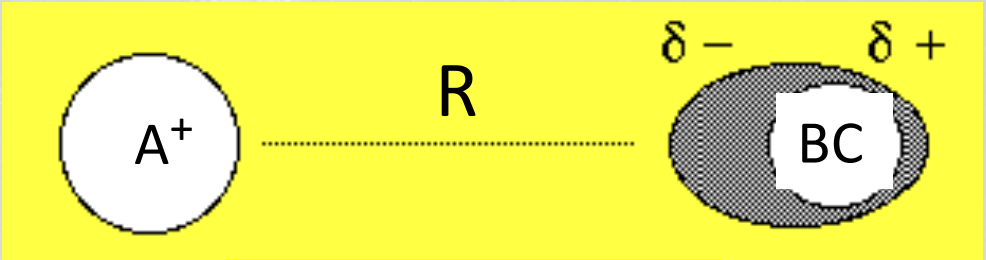
$$k \equiv \langle v \rangle \sigma_{NN} \approx 10^{-11/12} cm^3 s^{-1}$$

reaction rate coefficient

b. ion-neutral reactions

$$A^+ + BC \rightarrow AB^+ + C$$

Exothermic ion-molecule reactions are those that occur in cold gas because they do have significantly lower activation barriers thanks to the electrostatic attraction between the charged ion and the polar molecule (long-range induced ion-dipole atraction force (see Herbst & Klemperer 1973; Anicich & Huntress 1986)



attractive electrostatic i nteraction between the ion and dipole moment induced in the polar pa rticle

potential energy associated with the interaction → $V(R) = -\alpha e^2/2R^4$

Langevin reaction rate coefficient →

$$k \equiv \langle v \rangle \sigma_{IN} = 2\pi e \sqrt{\frac{\alpha}{\mu}} \approx 10^{-9} cm^3 s^{-1}$$

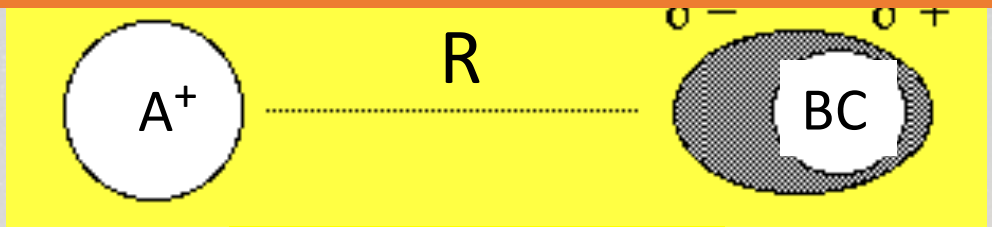
α = polarizability of neutral reactant
e = electronic charge
μ = reduced mass of colliding species

Langevin coefficient independent of T!

b. ion-neutral reactions

$$A^+ + BC \rightarrow AB^+ + C$$

Initiate the chemistry in cold molecular gas



attractive electrostatic i nteraction between the ion and dipole moment induced in the polariza ble particle

potential energy associated with the interaction → $V(R) = -\alpha e^2/2R^4$

Langevin reaction rate coefficient

$$k \equiv \langle v \rangle \sigma_{IN} = 2\pi e \sqrt{\frac{\alpha}{\mu}} \approx 10^{-9} cm^3 s^{-1}$$

α = polarizability of neutral reactant
e = electronic charge
μ = reduced mass of colliding species

Langevin coefficient independent of T!

Summary

1. Molecules in space
2. Detection of molecules
3. Formation of molecules:
   - Surface chemistry
   - Gas-phase chemistry
4. Complex organic chemistry

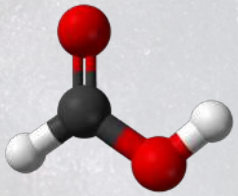
4. Complex organic chemistry

- Complex molecules are species with 6 or more atoms
- Complex organic Molecules: contain C
- First discovery of a complex organic molecule in space: methanol (CH_3OH) in 1970
- Some “exotic” molecules in interstellar clouds (most towards the Galactic Center, SgrB2):

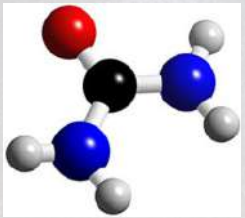
4. Complex organic chemistry

Some “exotic” molecules in interstellar clouds (most towards the Galactic Center, SgrB2):

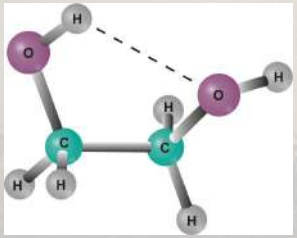
- formic acid (HCOOH)



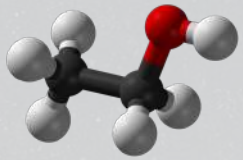
- urea (H_2NCONH_2)



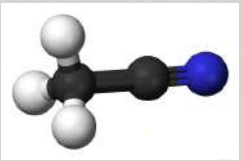
- ethylene glycol (a.k.a interstellar antifreeze) ($HOCH_2CH_2OH$)



- ethanol (CH_3CH_2OH)

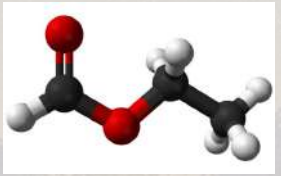


- methyl cyanide (CH_3CN)

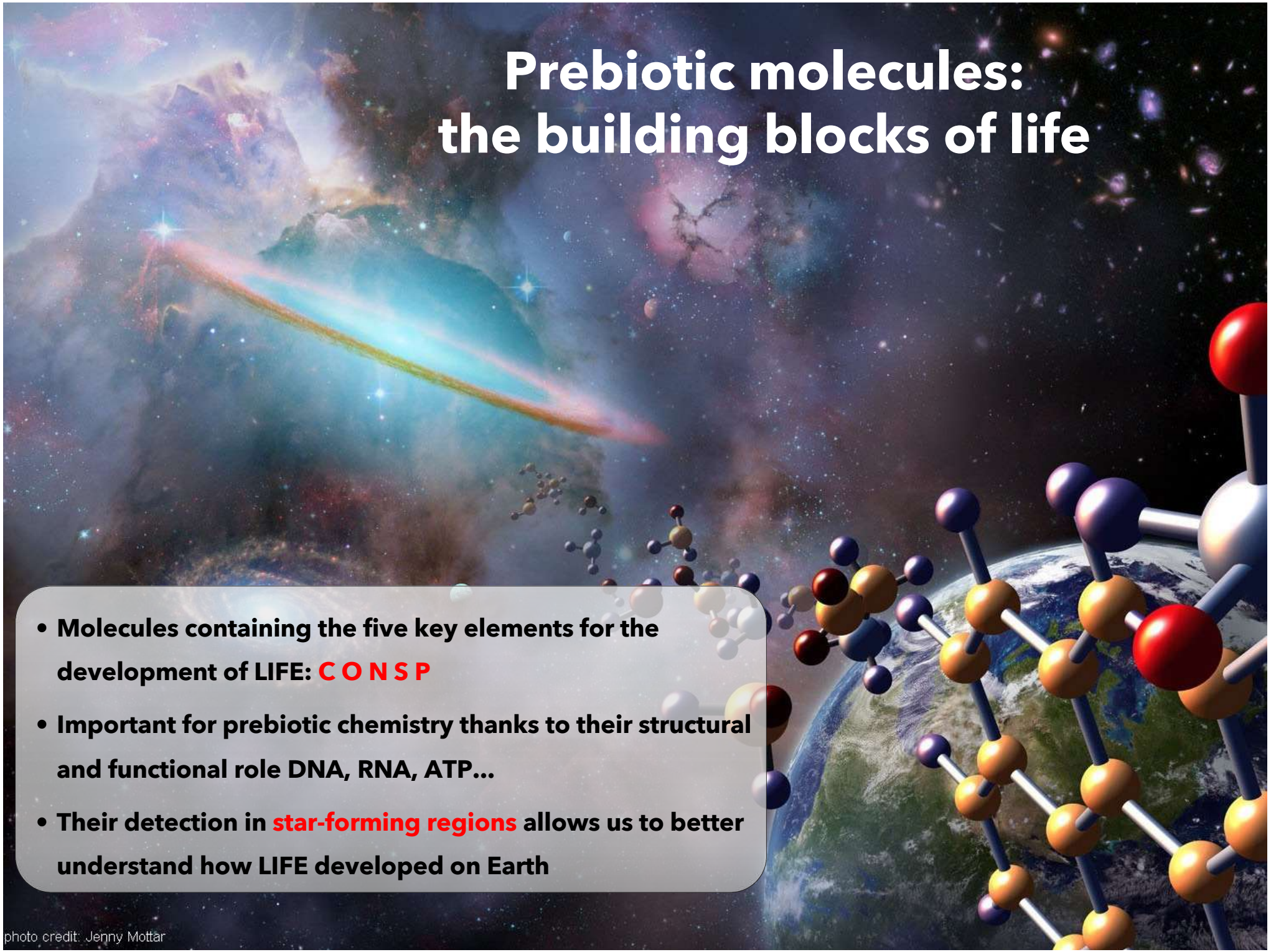


- acetone (CH_3COOCH_3)

- ethyl formate (C_2H_5OCHO) (flavour of berries)



Prebiotic molecules: the building blocks of life



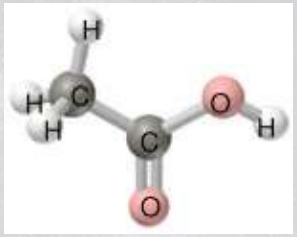
- Molecules containing the five key elements for the development of LIFE: **C O N S P**
- Important for prebiotic chemistry thanks to their structural and functional role DNA, RNA, ATP…
- Their detection in **star-forming regions** allows us to better understand how LIFE developed on Earth

photo credit: Jenny Mottar

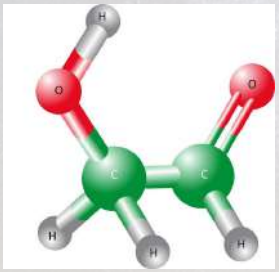
4. Complex organic chemistry

Prebiotic molecules: species biologically important because believed to be involved in the processes leading to the origin of life; building blocks of life

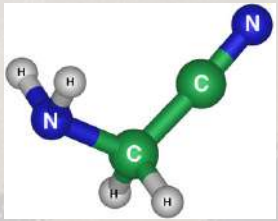
- acetic acid (vinegar) (CH_3COOH)



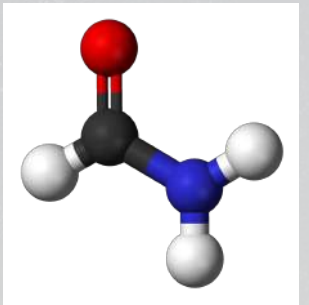
- glycolaldehyde (CH_2OHCHO)



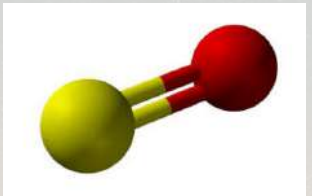
- amino acetonitrile (NH_2CH_2CN) (direct precursor of glycine??)

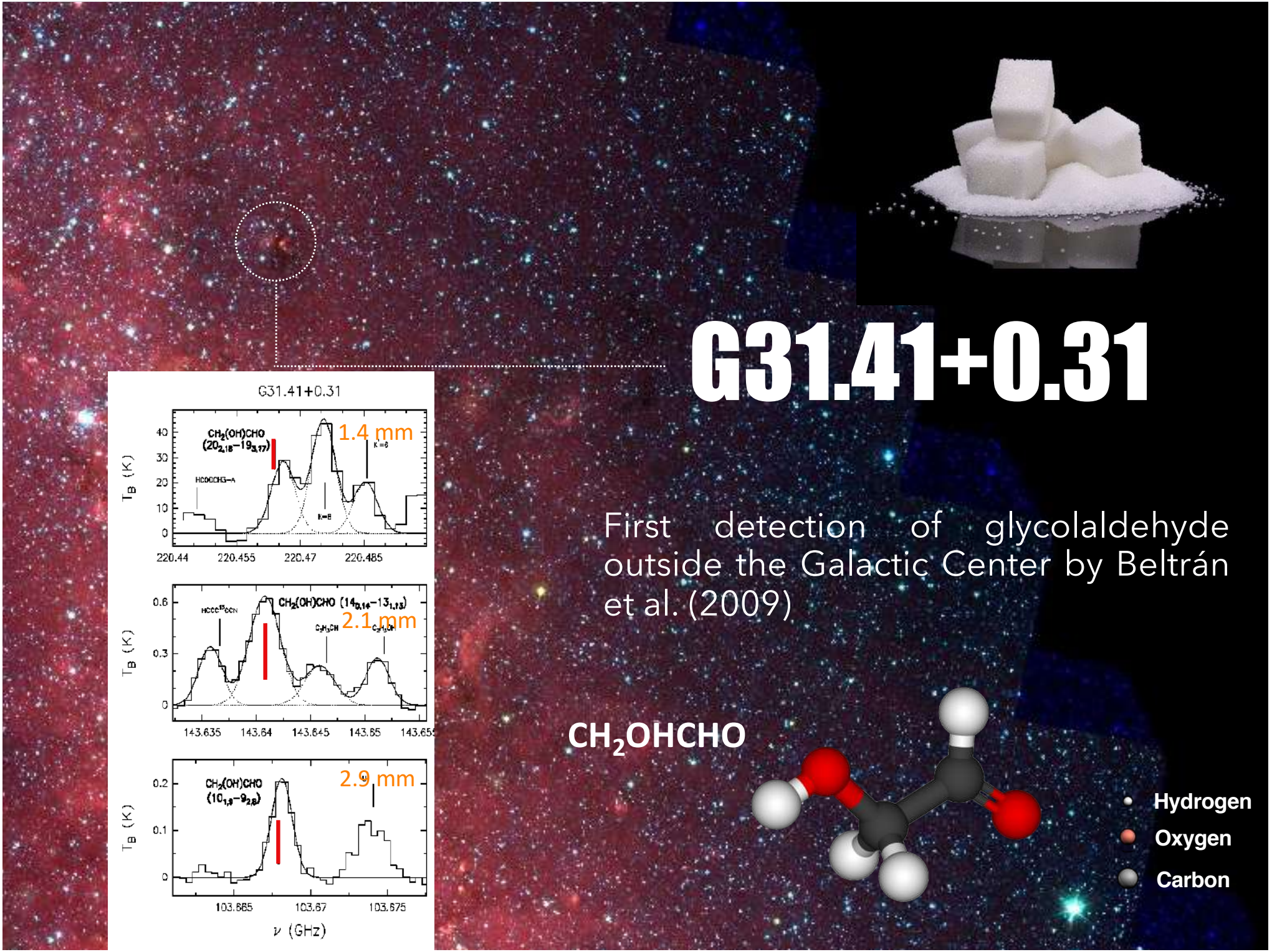


- formamide (NH_2COH)



- phosphorus monoxide (PO)

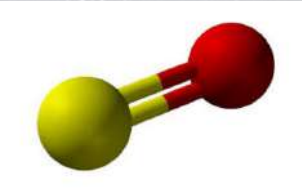




G31.41+0.31

First detection of glycolaldehyde outside the Galactic Center by Beltrán et al. (2009)

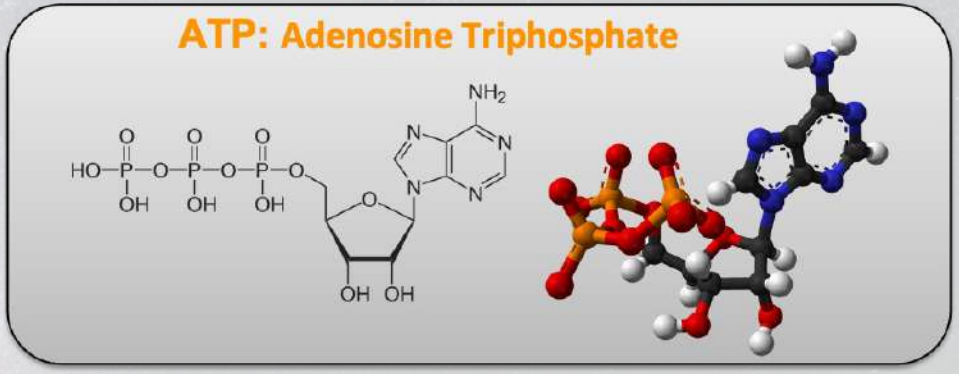
Phosphorus monoxide

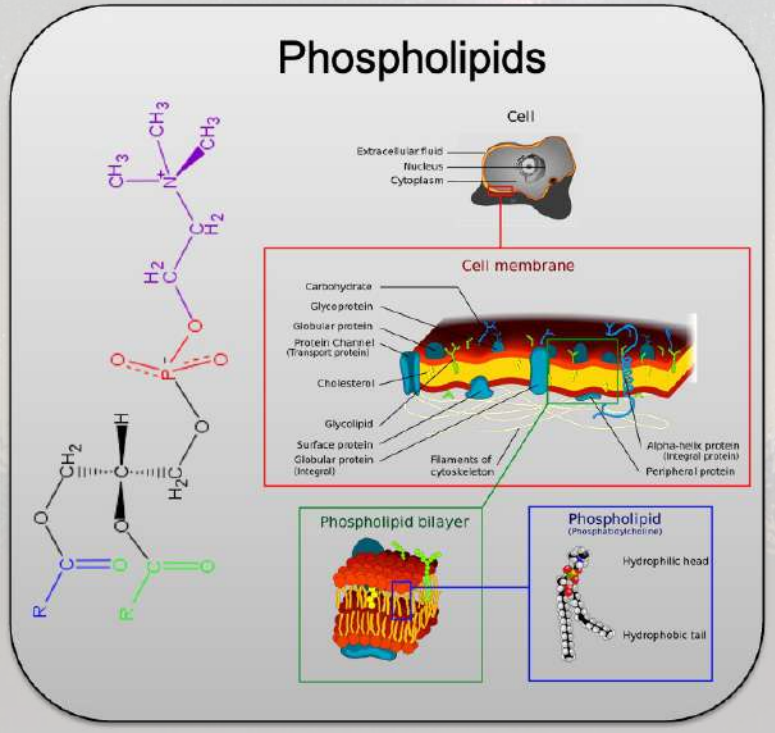


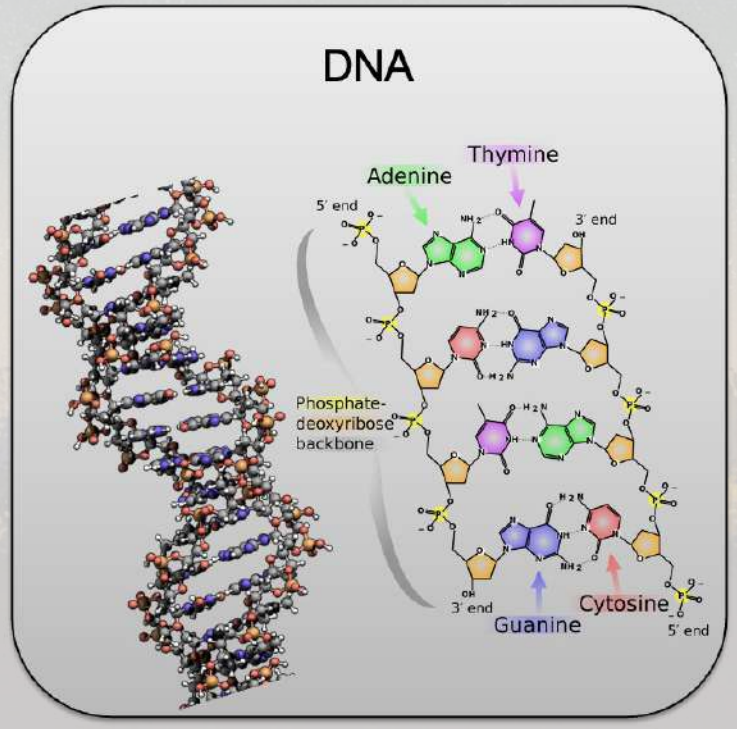
Phosphorus: key to Life

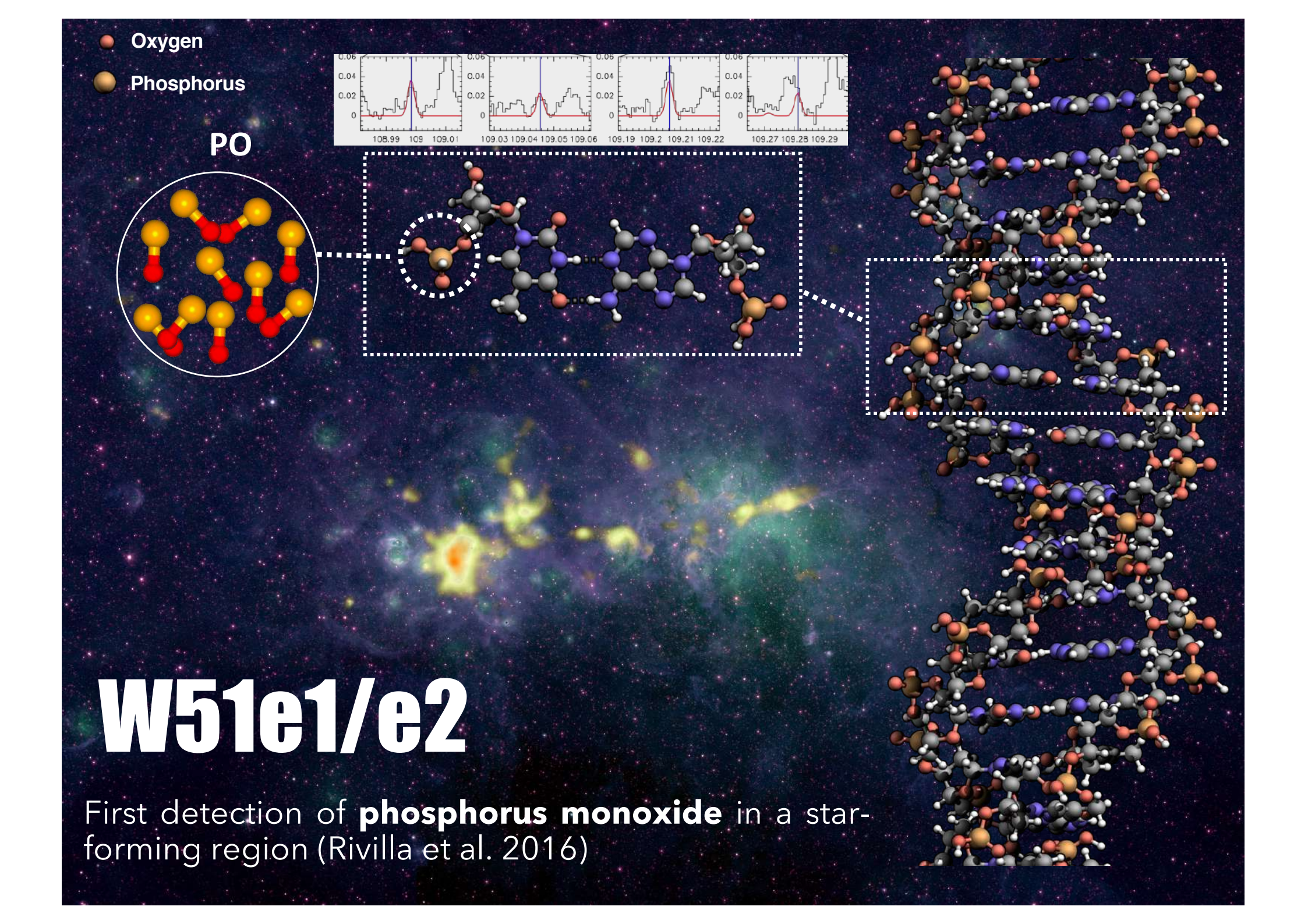
Chemical reactivity

Structural stability

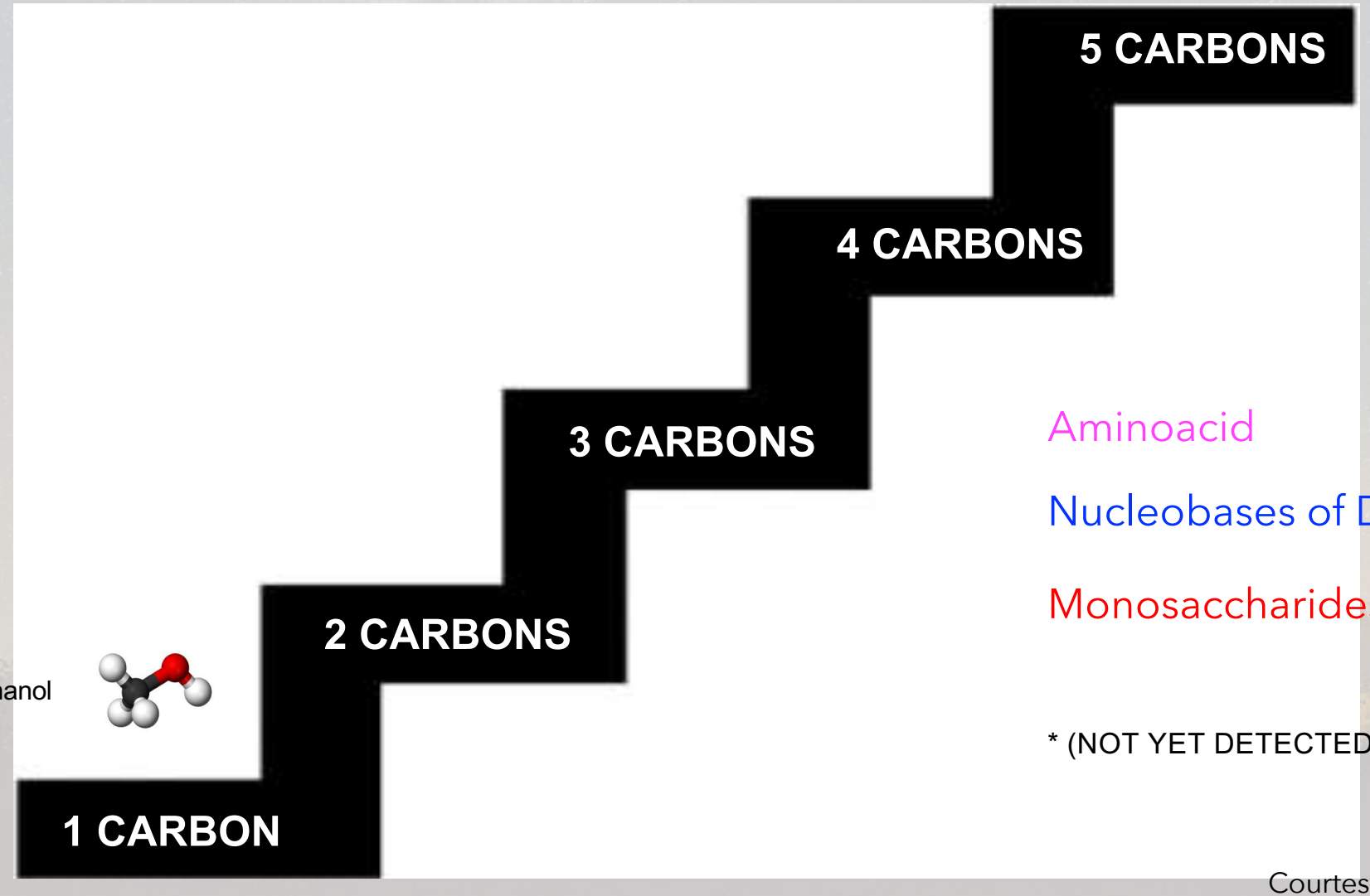






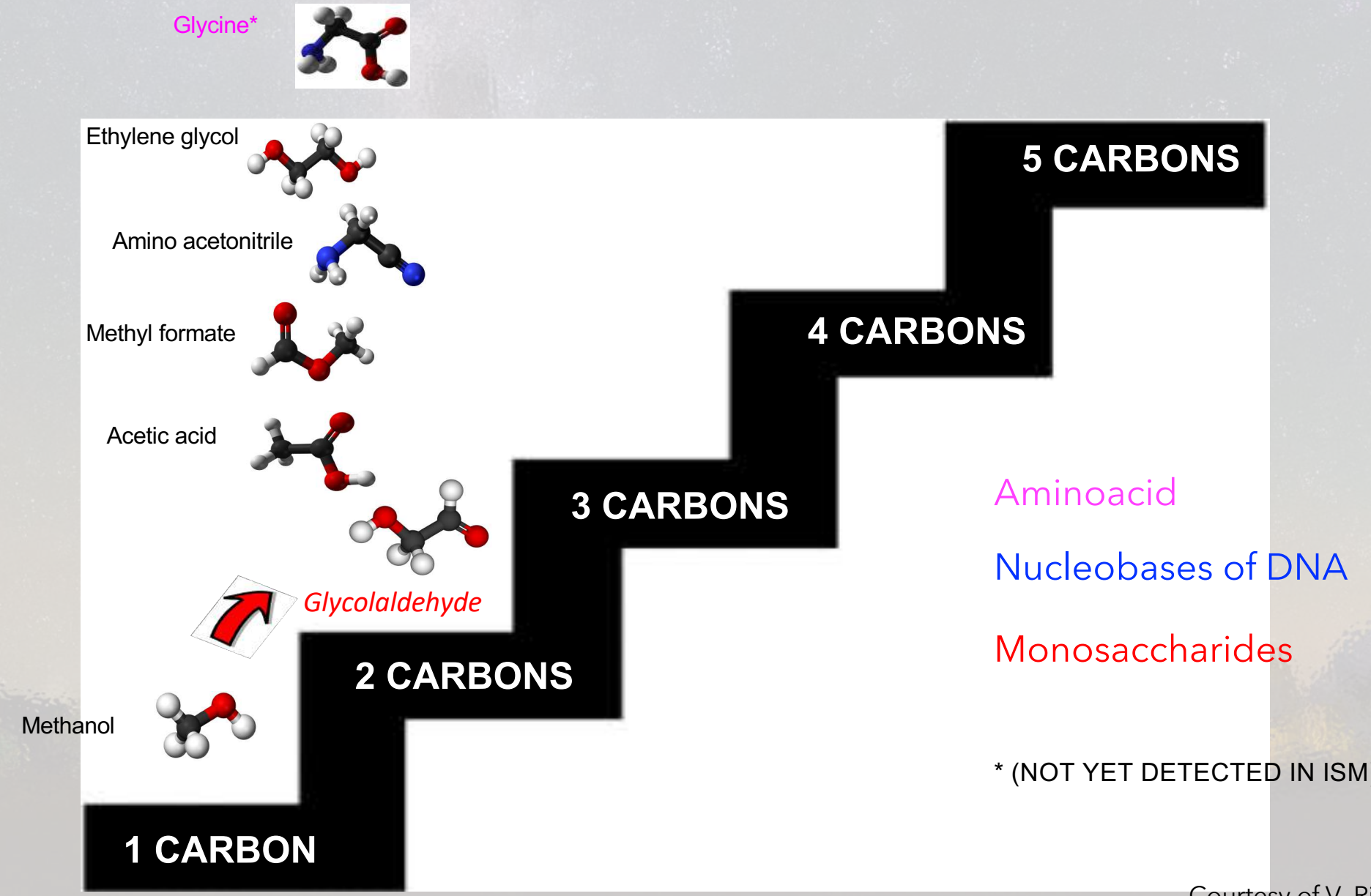

Oxygen
Phosphorus
PO
W51e1/e2
First detection of **phosphorus monoxide** in a star-forming region (Rivilla et al. 2016)

The chemical ladder of COMs



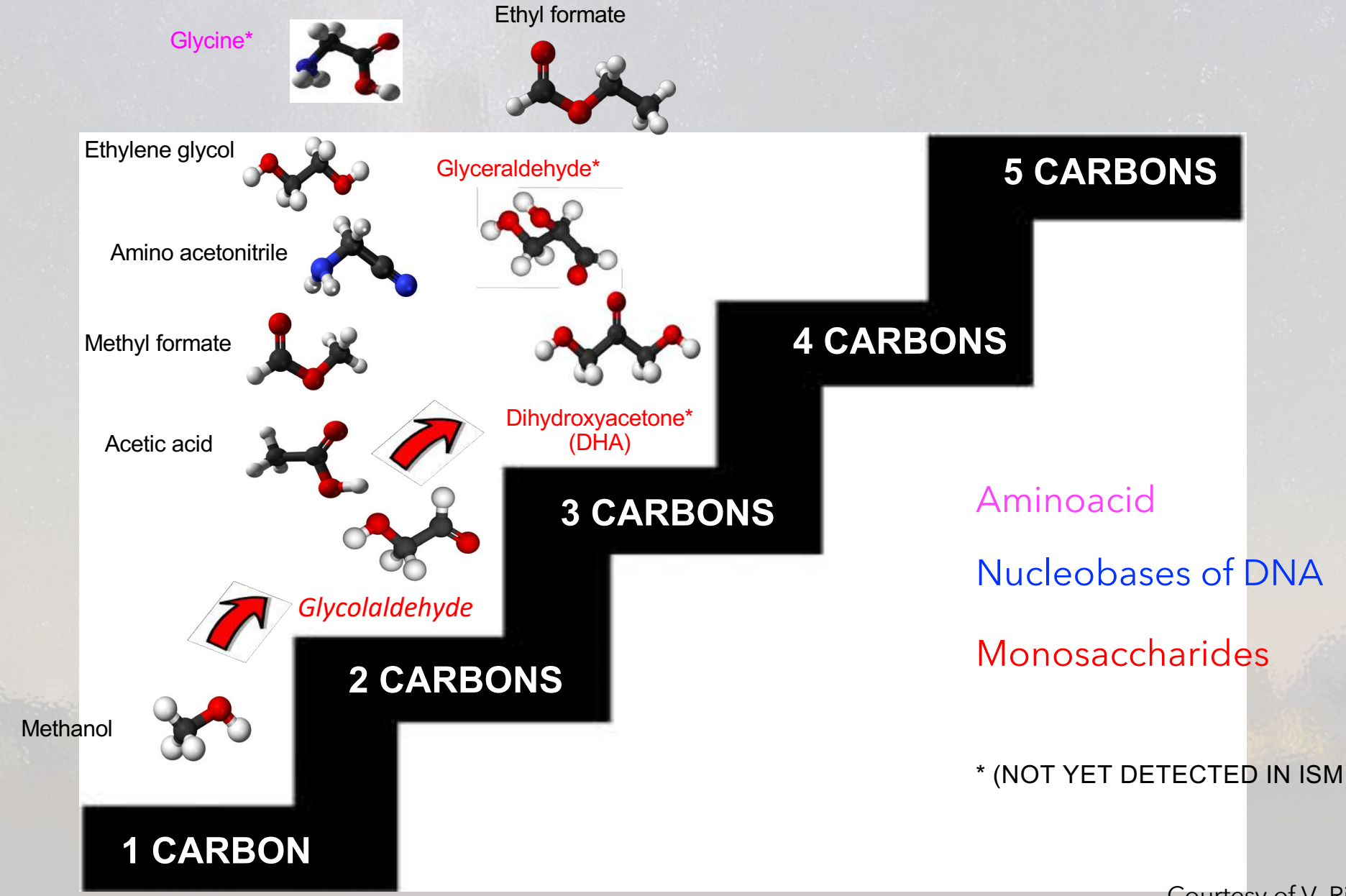
Courtesy of V. Rivilla

The chemical ladder of COMs



Courtesy of V. Rivilla

The chemical ladder of COMs



Aminoacid

Nucleobases of DNA

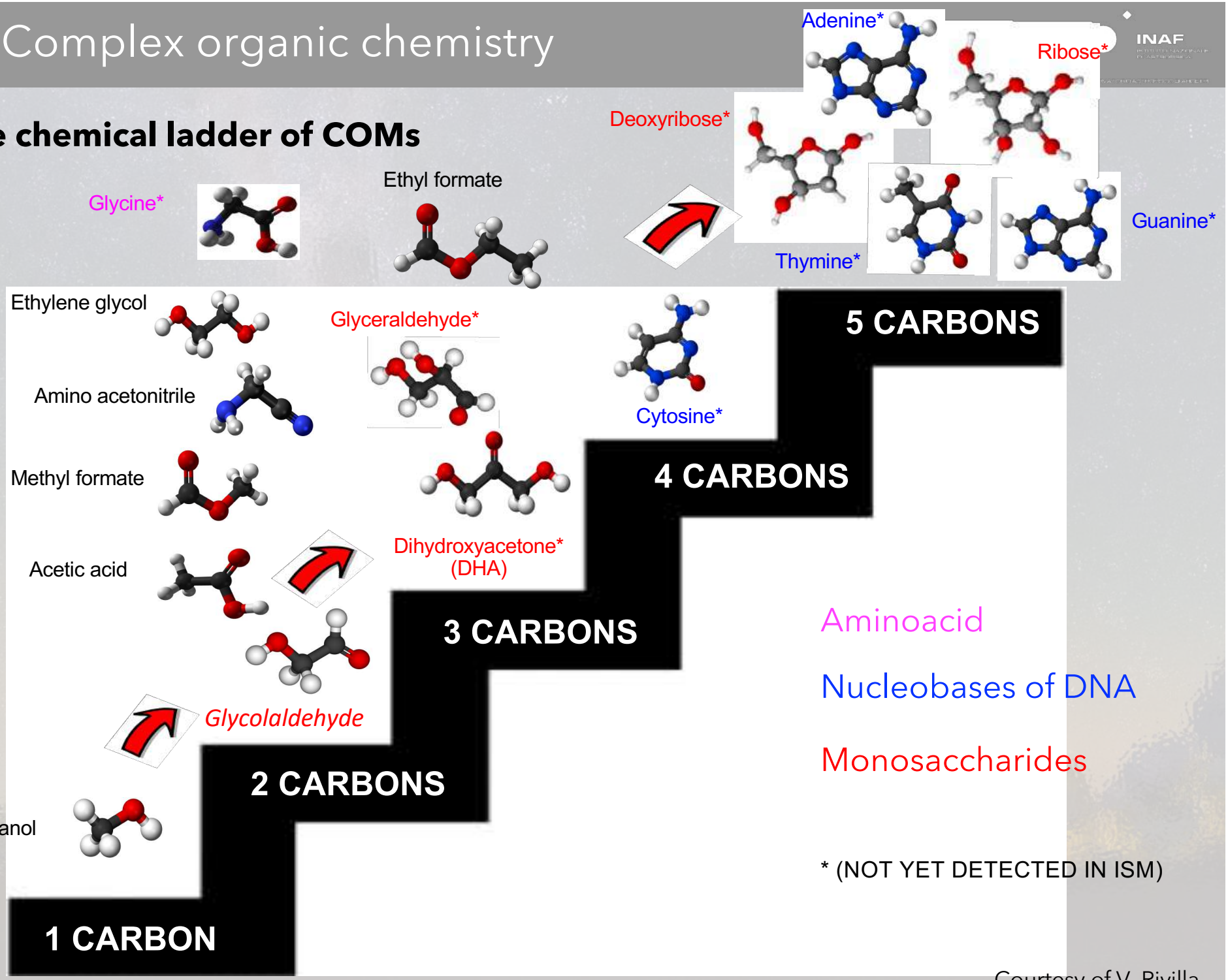
Monosaccharides

* (NOT YET DETECTED IN ISM)

Courtesy of V. Rivilla

4. Complex organic chemistry

The chemical ladder of COMs



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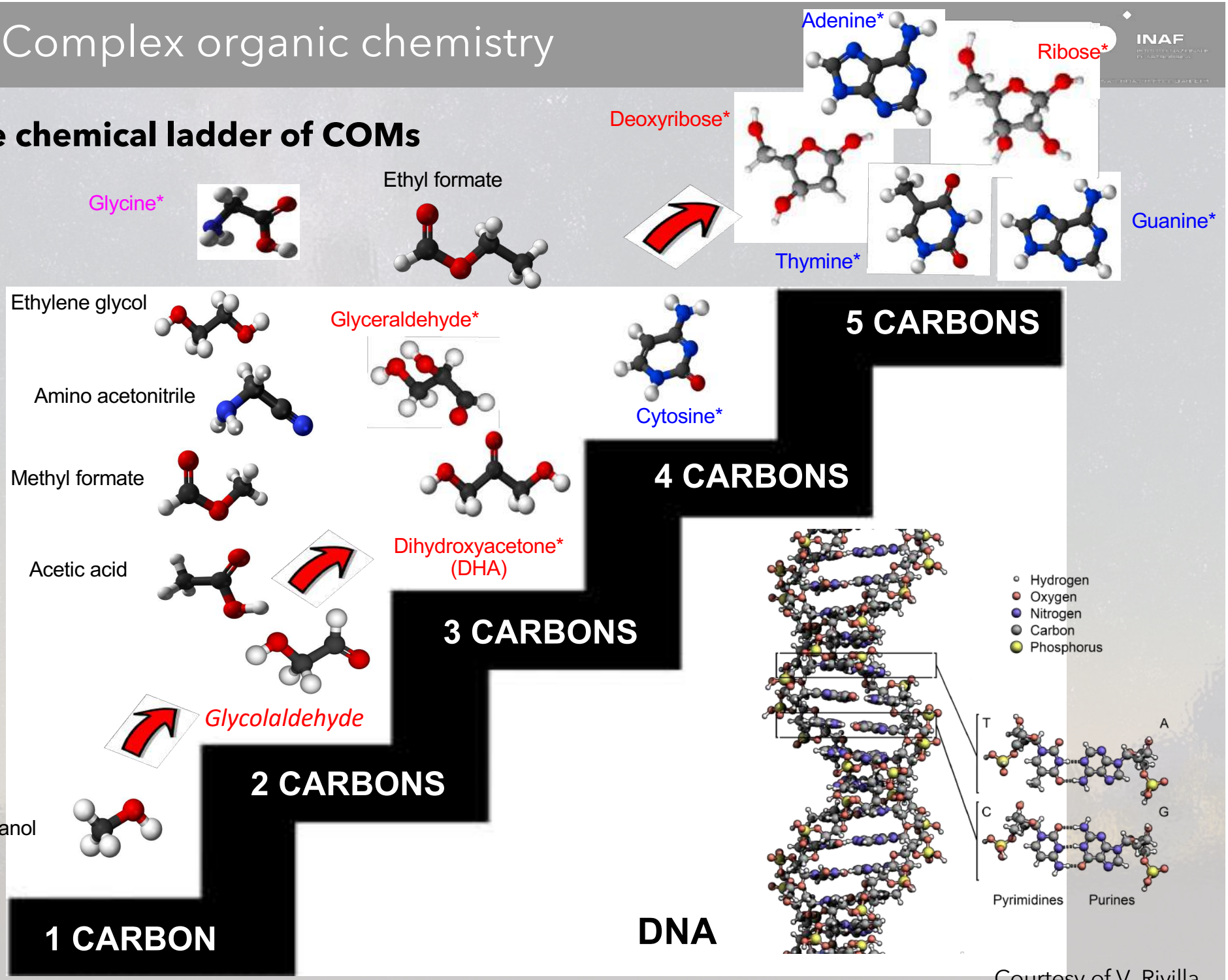
Courtesy of V. Rivilla

4. Complex organic chemistry

The chemical ladder of COMs

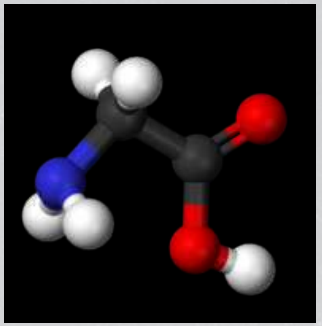


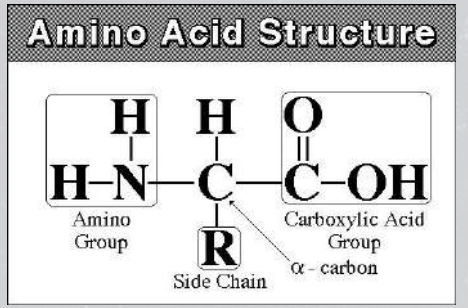
Courtesy of V. Rivilla

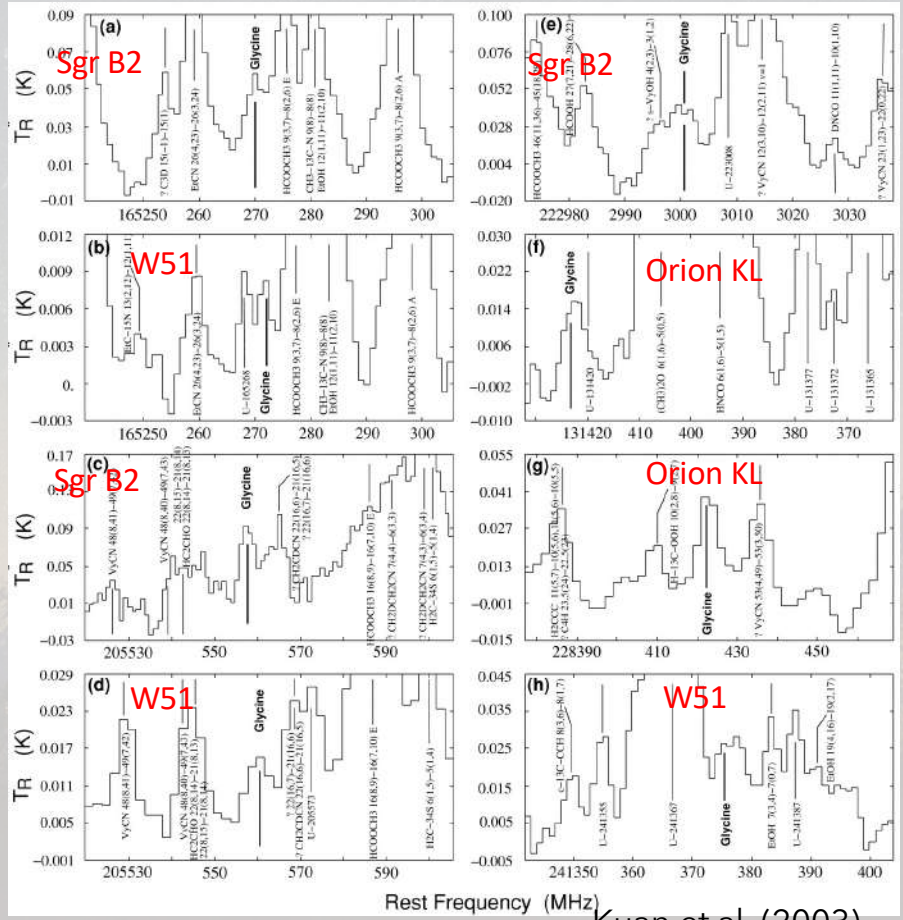
Glycine

- Glycine is the simplest of the 20 amino acids, building blocks of proteins and DNA
- Firm detections in meteorites (e.g. Ehrenfreundet al. 2001) and comets (Elsila et al. 2009)
- Searches in protostellar cores have NOT yielded any firm detection (Kuan et al. 2003, Snyder et al. 2005; Cunningham et al. 2007; Jones et al. 2007).
- Kuan et at. (2003) claimed to have detected 27 spectral lines of glycine in the hot cores Sgr B2(N), Orion KL, and W51 e1/e2. Snyder et al. (2005) disputed the claim and concluded that the identified lines are more likely due to weeds such as C_2H_5CN (ethyl cyanide), C_2H_3CN (vinyl cyanide), and *gauche*-ethanol.

NH_2CH_2COOH







Kuan et al. (2003)

What constitutes a firm detection

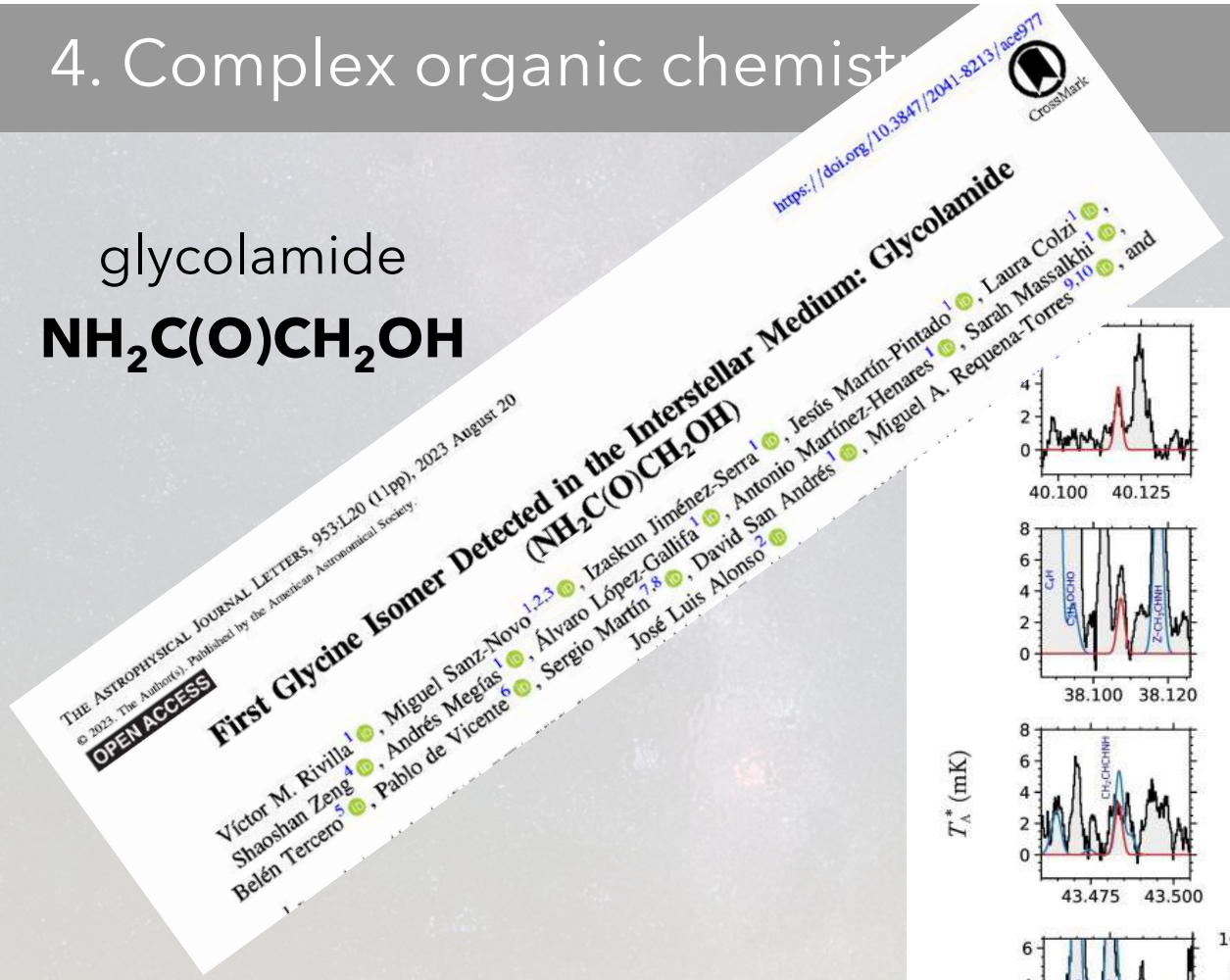
- The procedure for unequivocally identifying new molecules requires that at least the following first 3 criteria are met (Belloche et al. 2008; Snyder et al. 2005; Ziurys & Apponi 2005):

1) Rest frequencies are accurately known to 1:10^7, either from direct laboratory measurements or from a high-precision Hamiltonian model
2) Observed frequencies of clean, non-blended lines agree with rest frequencies for a single well-determined velocity of the source
3) All predicted lines of a molecule based on a LTE spectrum at a well-defined rotational temperature and appropriately corrected for beam dilution are present in the observed spectrum at roughly their predicted relative intensities. A single anti-coincidence (that is, a predicted line missing in the observational data) is a much stronger criterion for rejection than hundreds of coincidences are for identification.
4) Other criteria: to obtain interferometric images of the source and show that all lines of the new molecule originate from the same location.

4. Complex organic chemistry

glycolamide

$NH_2C(O)CH_2OH$



THE ASTROPHYSICAL JOURNAL LETTERS, 953:L20 (11pp), 2023 August 20
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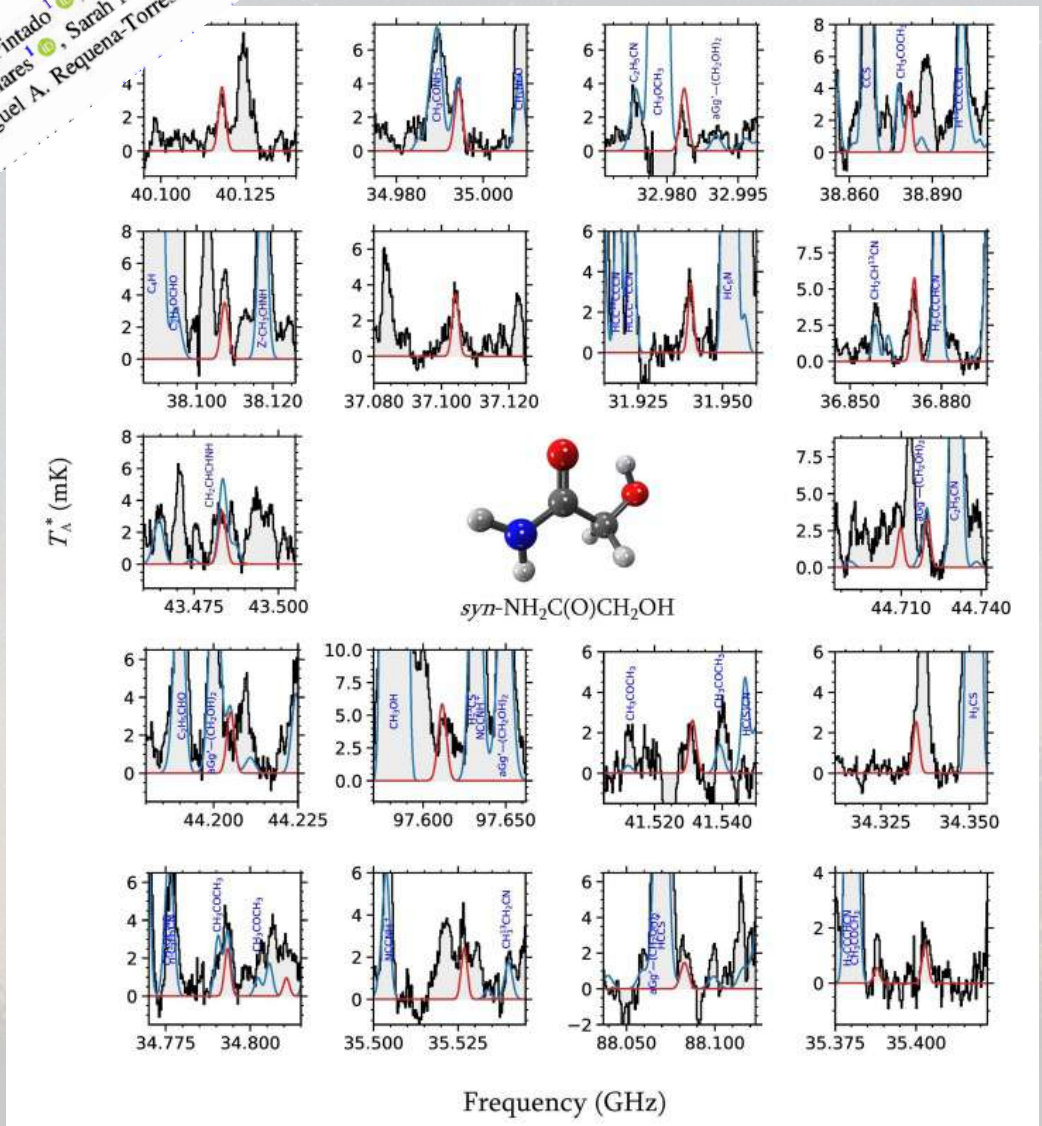
https://doi.org/10.3847/2041-8213/ace977

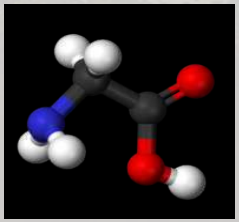
First Glycine Isomer Detected in the Interstellar Medium: Glycolamide ($NH_2C(O)CH_2OH$)

Víctor M. Rivilla[1], Miguel Sanz-Novo[1,2,3], Izaskun Jiménez-Serra[1], Jesús Martín-Pintado[1], Laura Colzi[1], Shaoshan Zeng[4], Andrés Megías[1], Álvaro López-Gallifa[1], Antonio Martínez-Henares[1], Sarah Massalkhi[1], Belén Tercero[5], Pablo de Vicente[6], Sergio Martín[7,8], David San Andrés[1], Miguel A. Requena-Torres[9,10], and José Luis Alonso[2]

G+0.693–0.027



glycine



NH_2CH_2COOH

Rivilla et al. (2023)

4. Complex organic chemistry

Complex organic molecules have been detected from prestellar to protostellar objects:

LOW MASS: recommended reading Caselli & Ceccarelli (2012)

- prestellar cores
- hot corinos
- circumstellar disks
- molecular outflows (shocks)

HIGH MASS: recommended reading J. Jorgensen, A. Belloche, R.T. Garrod (2020)

- IRDCs
- hot molecular cores
- circumstellar disks

4. Complex organic chemistry

Complex organic molecules have been detected from prestellar to protostellar objects:

LOW MASS: recommended reading Caselli & Ceccarelli (2012)

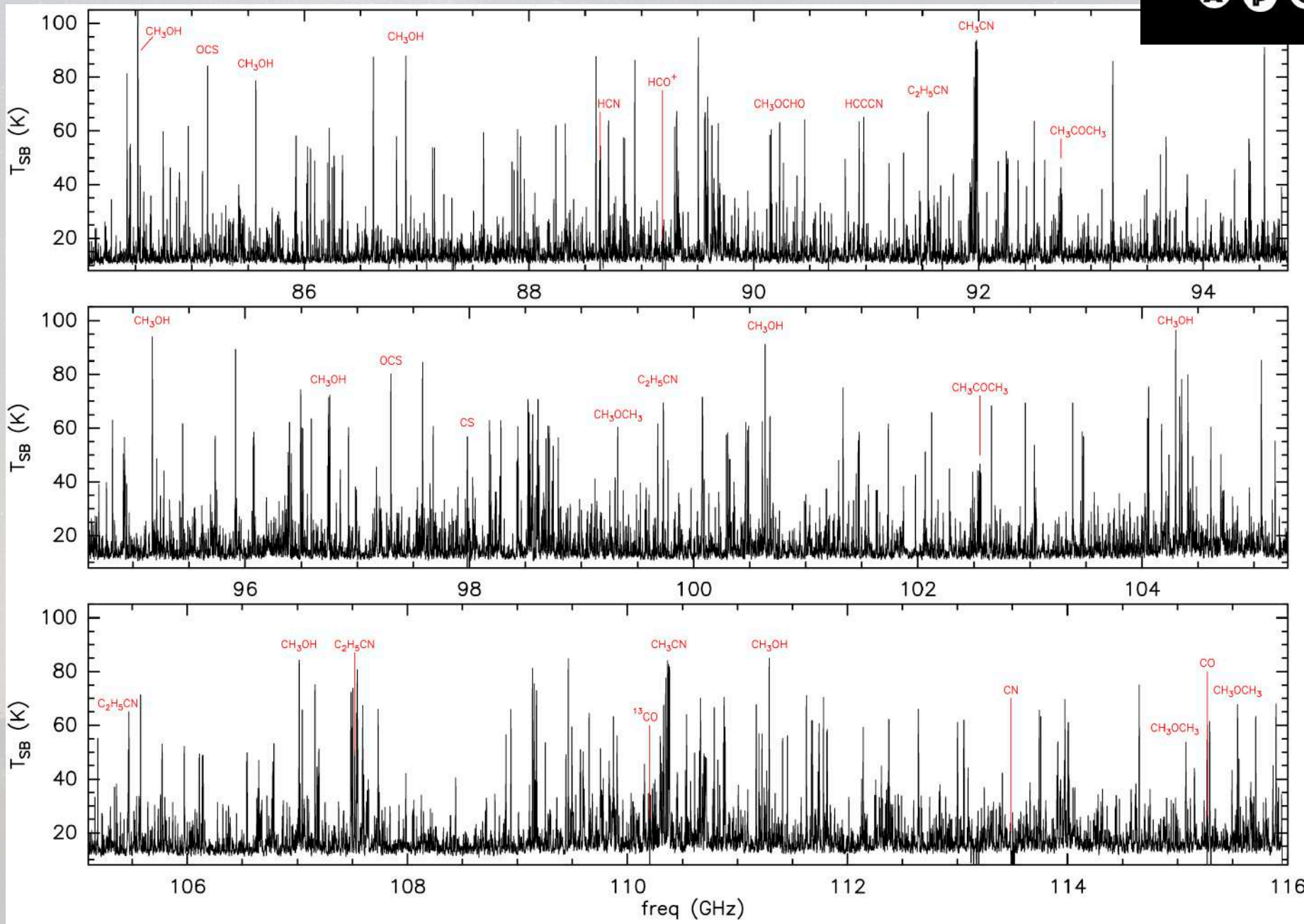
- prestellar cores
- hot corinos
- circumstellar disks
- molecular outflows (shocks)

HIGH MASS: recommended reading J. Jorgensen, A. Belloche, R.T. Garrod (2020)

- IRDCs
- hot molecular cores: most rich reservoirs of COMs in the MW
  Also in the Magellanic Clouds (SMC) (Sewilo et al. 2019)
- circumstellar disks

4. Complex organic chemistry

GUAPOS: unbiased ALMA Band 3 survey of G31.41+0.31



Mininni+ (2020)

4. Complex organic chemistry

FORMATION MECHANISM in HOT SOURCES

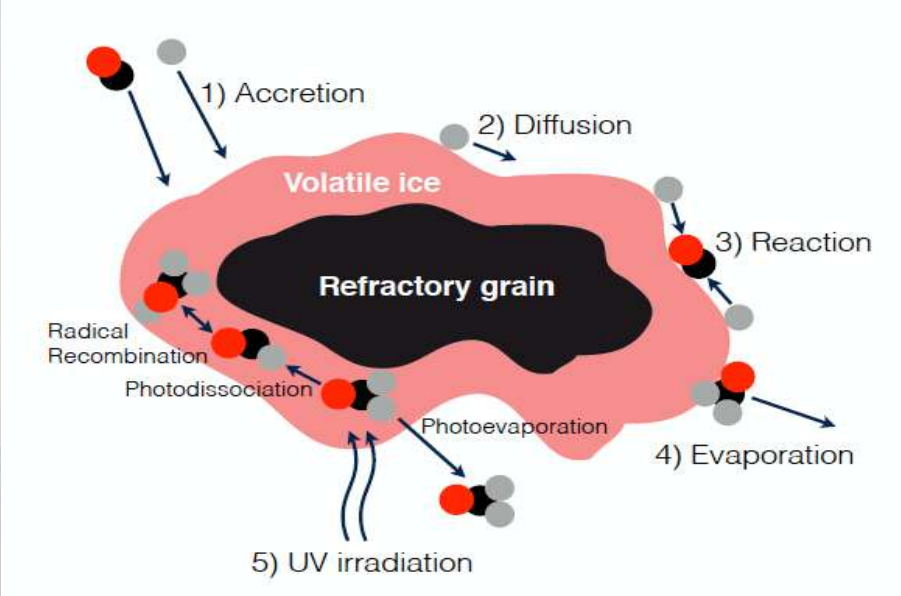
1. Grain-surface chemistry: COMs are formed on ices and then released into the gas phase

2. Gas-phase chemistry: COMs are daughter species, i.e. are formed in gas-phase following the release of parent species such as methanol and formaldehyde? (T~100 K)

FORMATION MECHANISM in HOT SOURCES

COMs mainly formed via surface are formed on ices and then released into the gas phase

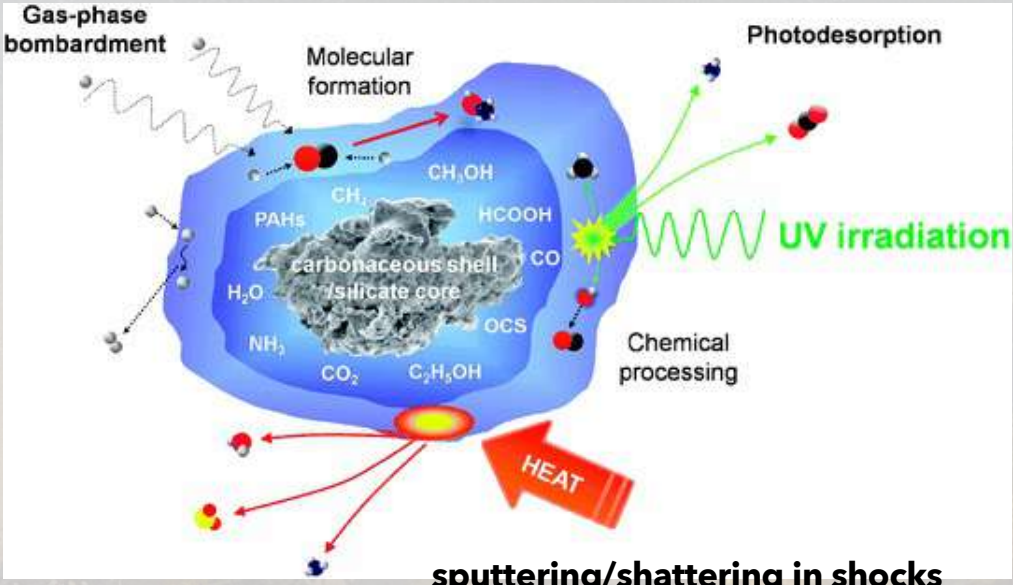
1. Hydrogenation (H addition; Charnley et al. 1997, 2001)
2. Radical-radical surface reactions (efficient at T>30 K; Garrod et al. 2008)



FORMATION MECHANISM in HOT SOURCES

- Cold gas in the ISM 'made up' of simple molecules (e.g. CO, HCN, N_2, O_2, etc) frozen onto dust grains
- Accretion of atoms and molecules on dust + surface reactions form more complex molecules: CO_2, CH_3OH, H_2O etc (ices)
- Back into the gas phase when dust heats up (e.g. by a star) → fast neutral-neutral and ion-neutral reactions → larger complex organic molecules
- Production of organic molecules can be enriched by thermal and energetic processing (UV and cosmic rays) in the gas phase (and possibly in the solid phase)

cosmic-ray desorption



sputtering/shattering in shocks

thermal desorption

Burke & Brown (2010)

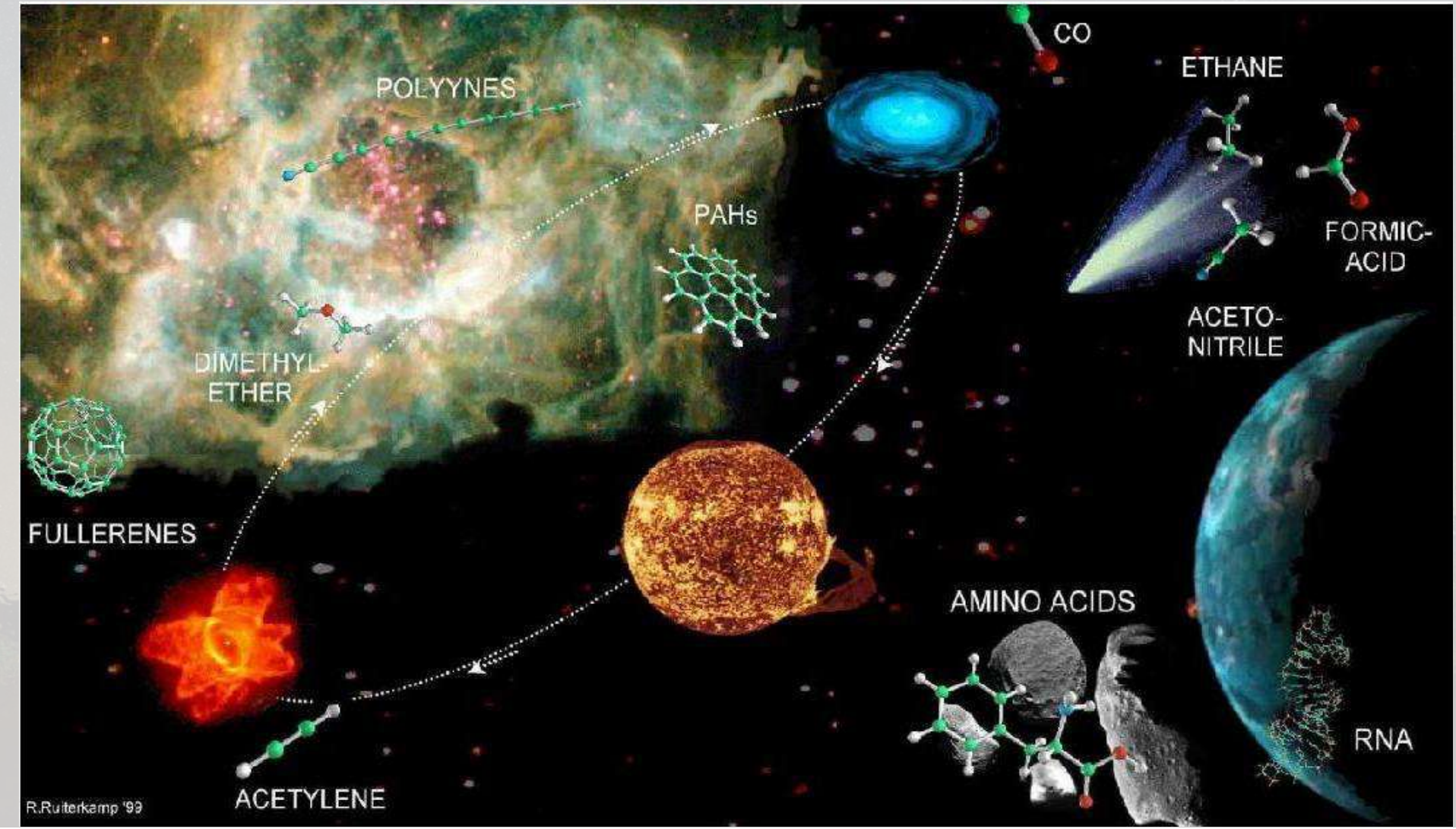
FORMATION MECHANISM in COLD SOURCES

Radical-radical surface formation inefficient at T< 30 K

New mechanisms proposed:

1. Gas phase formation (Vasyunin & Herbst 2013; Balucani+2015; Vasyunin+2017)
2. Non-canonical explosions (Rawlings et al. 2013) (catastrophic recombination of atomic hydrogen)
3. Cosmic-ray induced radical diffusion (Reboussin et al. 2014)
4. Impulsive spot heating on grains (Ivlev et al. 2015) (local heating leads to chemical desorption triggered by the exothermic chemical reaction(s) between free radicals frozen in the bulk of ice)
5. Formation after H atom addition/abstraction on grains (Chuang et al. 2016)

Tools
Lecture 3b



1a. Molecular spectroscopy

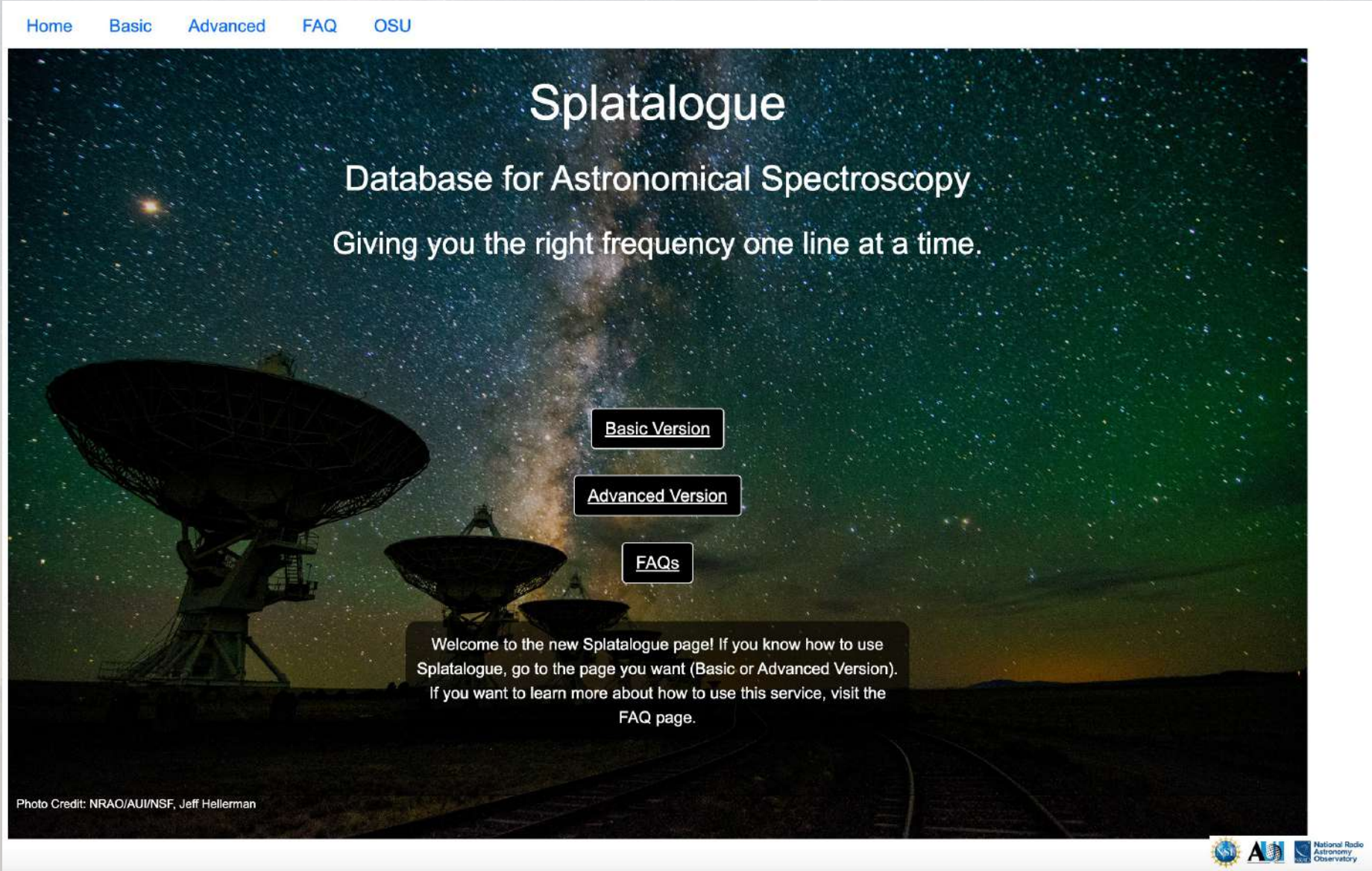
Atomic and molecular databases:

- NRAO – Splatalogue: https://splatalogue.online
- The Cologne Database for Molecular Spectroscopy (CDMS): https://cdms.astro.uni-koeln.de/cdms/portal/
- The JPL Cataloge: https://spec.jpl.nasa.gov/
- The Lovas Catalogue: https://physics.nist.gov/cgi-bin/micro/table5/start.pl

- Atomic fine structure lines: https://www.pa.uky.edu/~peter/newpage/
- HITRAN: https://hitran.org/
- NASA Ames Research Center Databases: http://www.astrochem.org/databases.php
- NIST Atomic Spectra Database: https://physics.nist.gov/PhysRefData/ASD/lines_form.html
- NIST frequency catalogue: https://webbook.nist.gov/chemistry/vib-ser/
- PAH Database (NASA Ames Research Center): https://www.astrochemistry.org/pahdb/theoretical/3.20/default/view

1a. Molecular spectroscopy

NRAO – Splatalogue:



1a. Molecular spectroscopy

NRAO – Splatalogue: Basic: Quick Picker: $H^{13}CO^+$ in ALMA Band 3

Photo Credit: NRAO/AUI/NSF

Search Species

e.g. ammonia, carbon, methanol, CO

Search Parameters

Quick Picker

CO v = 0	☐	^{13}CO v = 0	☐
$C^{17}O$	☐	$C^{18}O$	☐
CH_3OH v_t = 0	☐	H_2CO	☐
HCN v = 0	☐	HNC v = 0	☐
$H^{13}CN$ v = 0	☐	$HC^{15}N$ v = 0	☐
DCN v = 0	☐	HCO^+ v = 0	☐
CS	☐	$H^{13}CO^+$	☑
NH_3	☐	C I	☐
C II	☐	O I	☐
O III	☐	N II	☐
H_2O v = 0	☐	HDO	☐
SiO v = 0	☐	More molecules	

Save and Restore Settings

Settings Name

Save Restore

Query Filters

Telescope Bands

Any
ALMA Band 1 (35-50 GHz)
ALMA Band 3 (84-116 GHz)
ALMA Band 4 (125-163 GHz)

Energy Range

From To

E_L (K) E_U (K)

Specify a Frequency Range

From To

+ Frequency Range - Frequency Range

Frequency Unit GHz

Load Freqs From listobs

Choose files No file chosen

Astronomical Filters

None	◉
Top 20 list	○
Planetary Atmosphere	○
Hot Cores	○
Dark Clouds	○
Diffuse Clouds	○
Comets	○
AGB/PPN/PN	○
Extragalactic	○

Export Data

Export Fields

Export current fields	◉
Export current fields without Resolved QNs	○
Export CASA fields	○

Field Separator

Tab	◉
Colon	○

Range

All Records	◉
Current Page	○

Export

1a. Molecular spectroscopy

NRAO – Splatalogue: Basic: Quick Picker: $H^{13}CO^+$ in ALMA Band 3

Search Results

Search

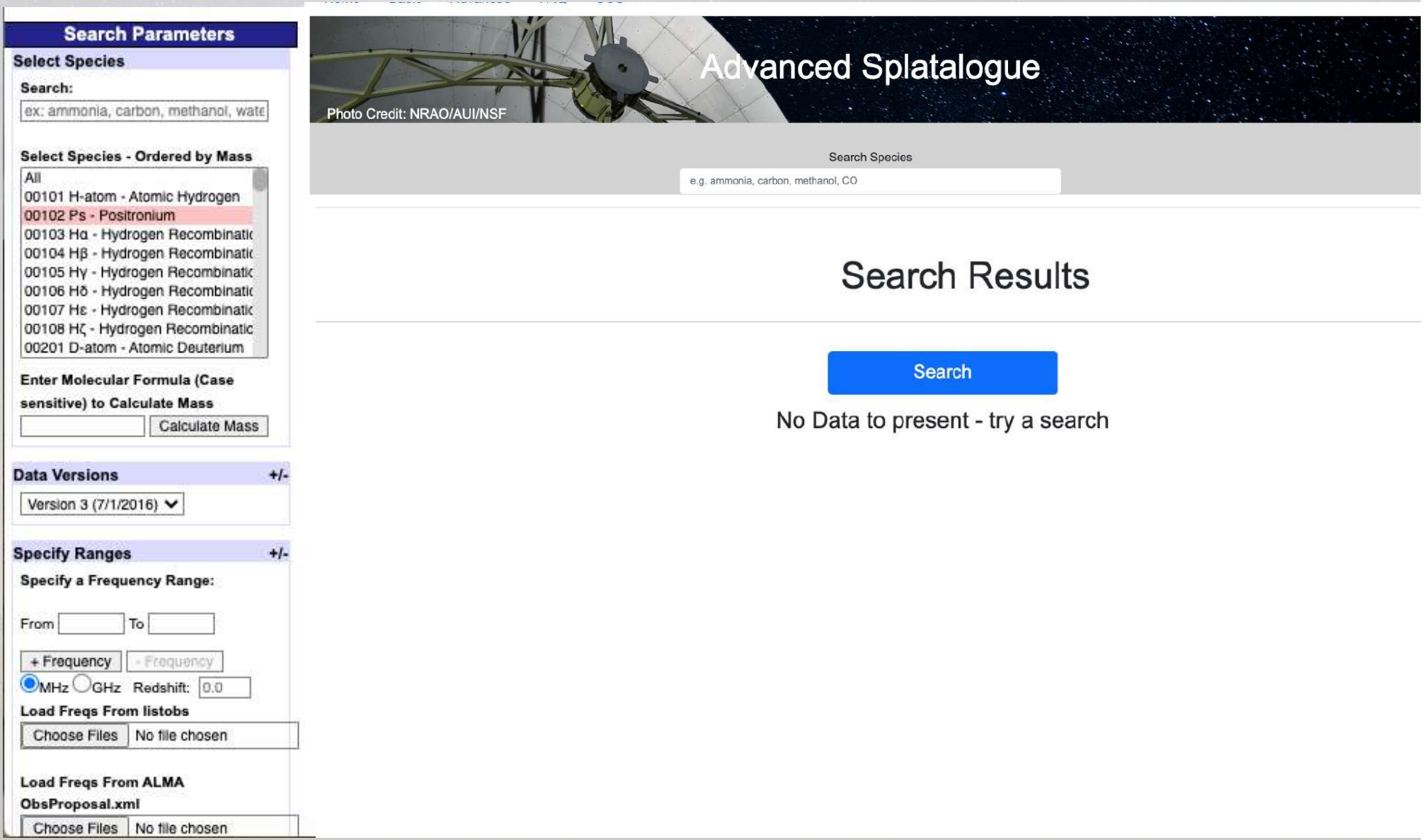
Found 68 lines
Query Limited to 670000 Rows
Showing lines 1 to 68
Previous Page Next Page

ALMA Band 1	ALMA Band 2	ALMA Band 3
ALMA Band 4	ALMA Band 5	ALMA Band 6
ALMA Band 7	ALMA Band 8	ALMA Band 9
ALMA Band 10		

#	Species	Chemical Name	Ordered Frequency (GHz) (rest frame, redshifted)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E_L(K)	E_U(K)	Linelist
1	$H^{13}CO^+$	Formylium	86.7542619, 86.7542619	J= 1- 0, F_1=1/2-1/2, F= 1- 1			0.000	4.16352	CDMS
2	$H^{13}CO^+$	Formylium	86.7542619, 86.7542619	J= 1- 0, F_1=1/2-1/2, F= 1- 1			0.000	4.16352	CDMS
3	$H^{13}CO^+$	Formylium	86.7542884, 86.7542884	1- 0			0.000	4.16353	CDMS
4	$H^{13}CO^+$	Formylium	86.7543004, 86.7543004	J= 1- 0, F_1=3/2-1/2, F= 2- 1			0.000	4.16353	CDMS
5	$H^{13}CO^+$	Formylium	86.7543014, 86.7543014	J= 1- 0, F_1=3/2-1/2, F= 1- 1			0.000	4.16353	CDMS
6	$H^{13}CO^+$	Formylium	86.7543014, 86.7543014	J= 1- 0, F_1=3/2-1/2, F= 1- 1			0.000	4.16353	CDMS
7	$H^{13}CO^+$	Formylium	86.7543029, 86.7543029	J= 1- 0, F_1=1/2-1/2, F= 0- 1			0.000	4.16353	CDMS
8	$H^{13}CO^+$	Formylium	173.5066501, 173.5066501	J= 2- 1, F_1=3/2-3/2, F= 2- 2			4.16351	12.49047	CDMS
9	$H^{13}CO^+$	Formylium	173.5066812, 173.5066812	J= 2- 1, F_1=3/2-1/2, F= 1- 0			4.16351	12.49047	CDMS
10	$H^{13}CO^+$	Formylium	173.5066826, 173.5066826	J= 2- 1, F_1=3/2-3/2, F= 1- 1			4.16351	12.49047	CDMS
11	$H^{13}CO^+$	Formylium	173.5066887, 173.5066887	J= 2- 1, F_1=3/2-1/2, F= 2- 1			4.16351	12.49047	CDMS
12	$H^{13}CO^+$	Formylium	173.5067003, 173.5067003	2- 1			4.16351	12.49047	CDMS
13	$H^{13}CO^+$	Formylium	173.5067081, 173.5067081	J= 2- 1, F_1=5/2-3/2, F= 3- 2			4.16351	12.49047	CDMS
14	$H^{13}CO^+$	Formylium	173.506712, 173.506712	J= 2- 1, F_1=5/2-3/2, F= 2- 1			4.16351	12.49047	CDMS
15	$H^{13}CO^+$	Formylium	173.506713, 173.506713	J= 2- 1, F_1=5/2-3/2, F= 2- 2			4.16351	12.49047	CDMS
16	$H^{13}CO^+$	Formylium	173.5067222, 173.5067222	J= 2- 1, F_1=3/2-1/2, F= 1- 1			4.16351	12.49047	CDMS
17	$H^{13}CO^+$	Formylium	260.2552753, 260.2552753	J= 3- 2, F_1=5/2-5/2, F= 3- 3			12.49053	24.98074	CDMS
18	$H^{13}CO^+$	Formylium	260.2553067, 260.2553067	J= 3- 2, F_1=5/2-5/2, F= 2- 2			12.49053	24.98074	CDMS
19	$H^{13}CO^+$	Formylium	260.2553333, 260.2553333	J= 3- 2, F_1=5/2-3/2, F= 3- 2			12.49053	24.98074	CDMS
20	$H^{13}CO^+$	Formylium	260.2553361, 260.2553361	J= 3- 2, F_1=5/2-3/2, F= 2- 1			12.49053	24.98074	CDMS
21	$H^{13}CO^+$	Formylium	260.255339, 260.255339	3- 2			12.49053	24.98074	CDMS

1a. Molecular spectroscopy

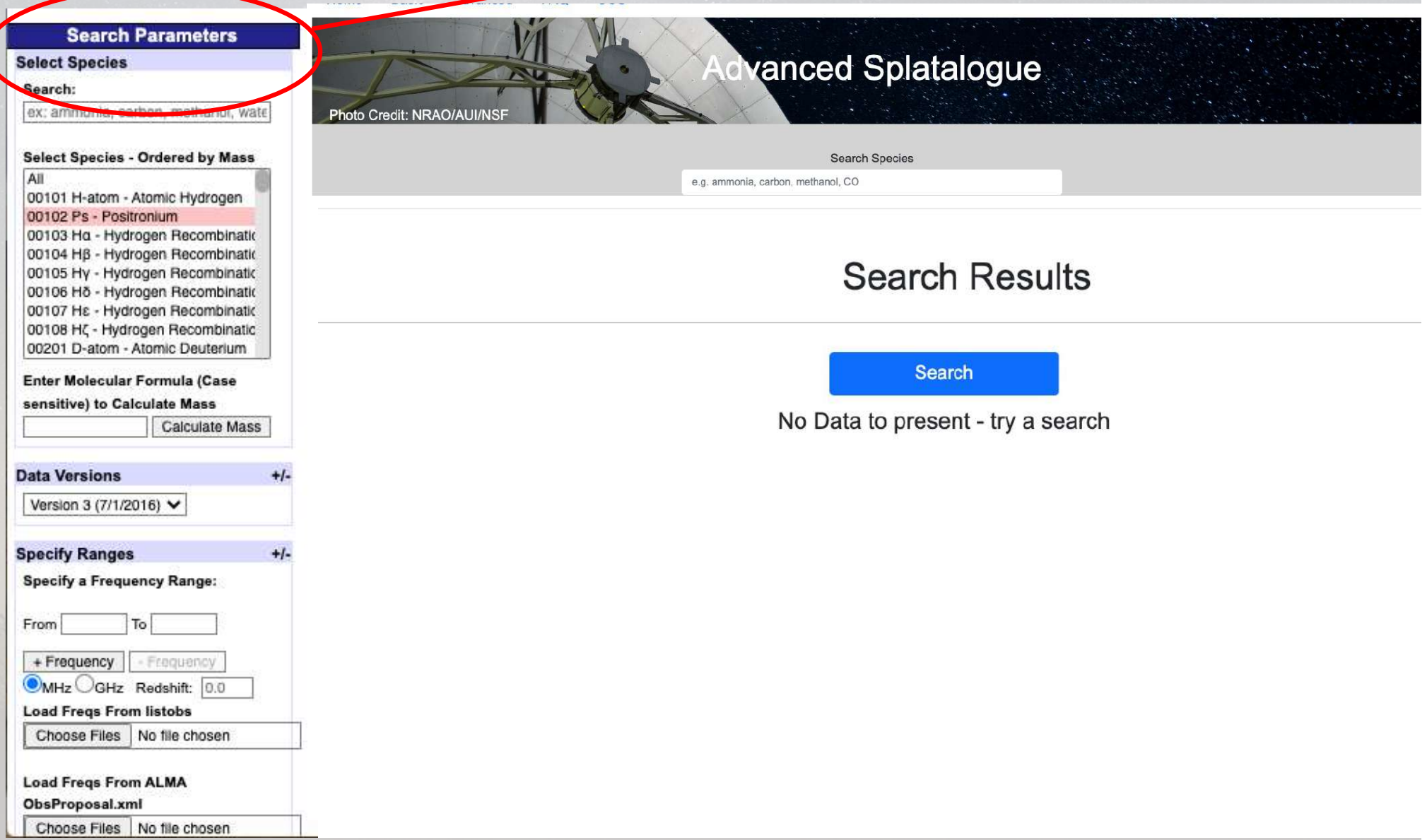
NRAO – Splatalogue: Advanced



1a. Molecular spectroscopy

NRAO – Splatalogue: Advanced

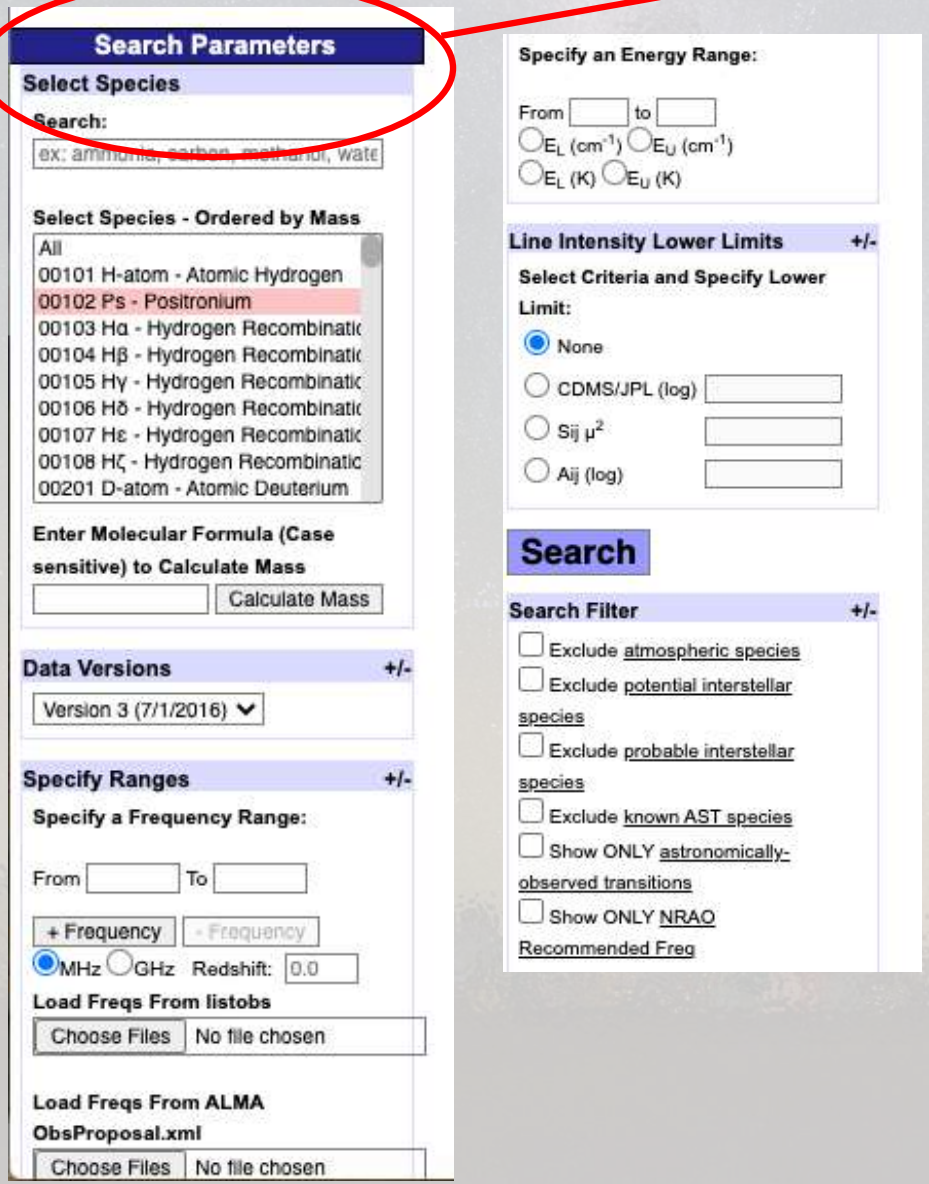
Search Parameters



1a. Molecular spectroscopy

NRAO – Splatalogue: Advanced

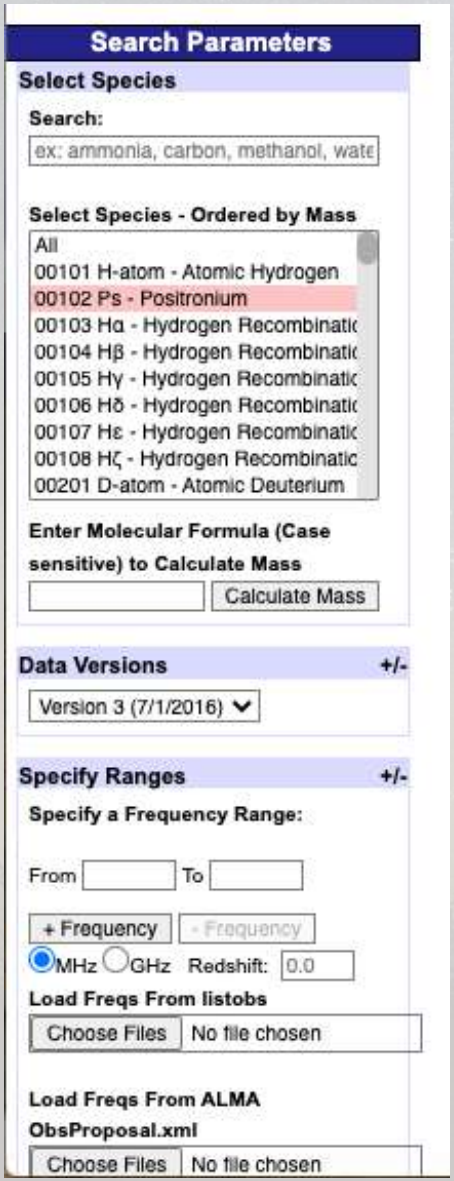
Search Parameters

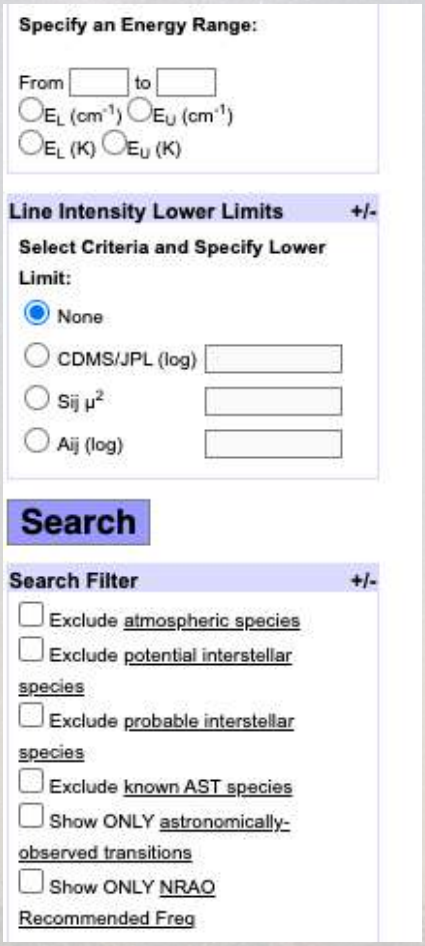


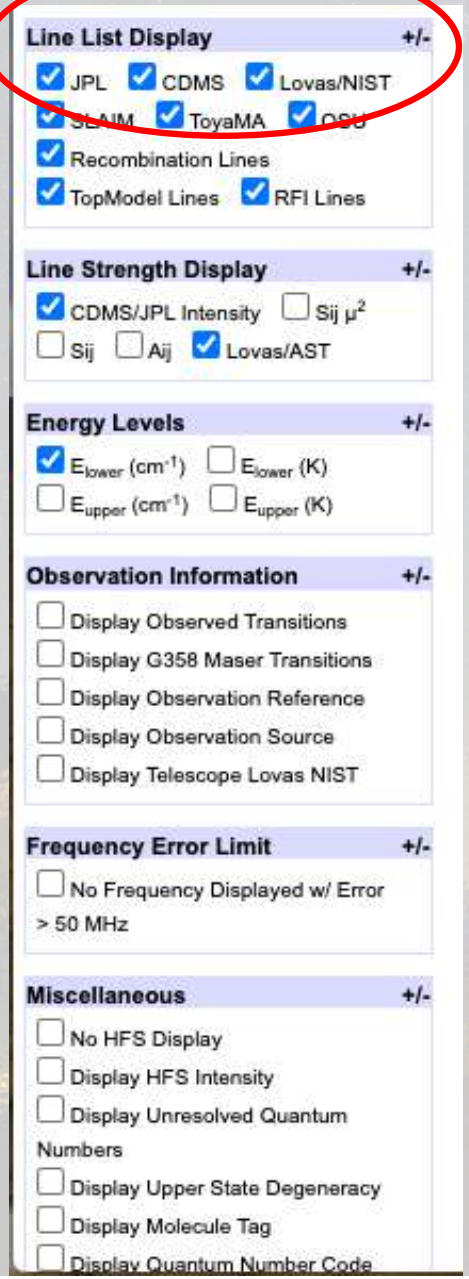
1a. Molecular spectroscopy

Line list Display

NRAO – Splatalogue: Advanced



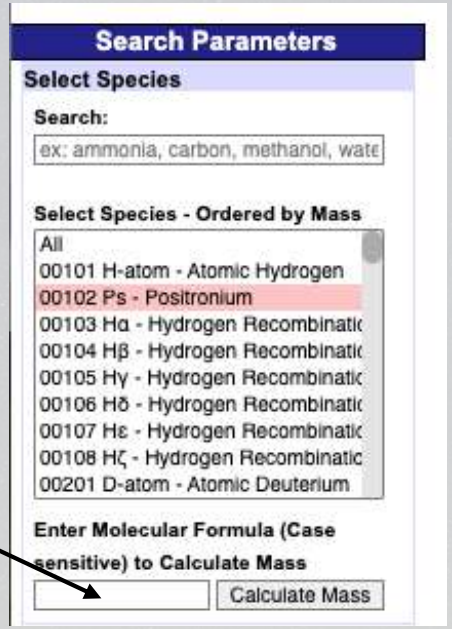




NRAO – Splatalogue: Advanced

Search parameters:

1. Select species:
   by name, or using formula calculate molar mass



Species are colored by their status as astronomical molecules. The color coding is:

WHITE: Known astronomical molecules
RED: Possible astronomical molecules
BLUE: Atmospheric molecules
GREEN: Probable astronomical molecules – commonly, excited vibrational states and isotopologues of known molecules

NRAO – Splatalogue: Advanced

Search parameters:

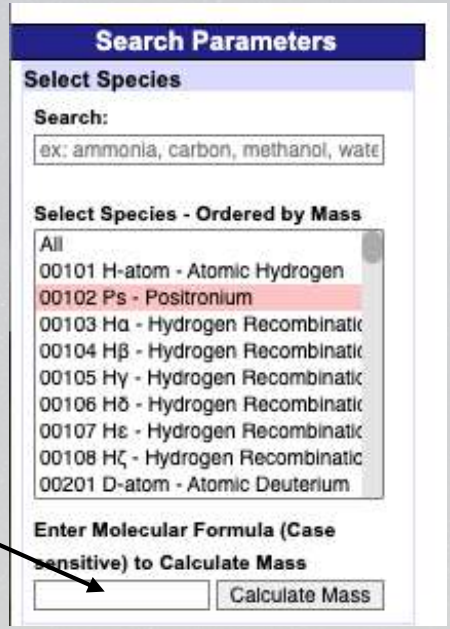
1. Select species:
   by name, or using formula calculate mass

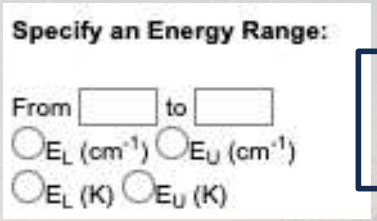
2. Frequency range:
   in MHz, GHz, or redshift

3. Specify an energy range:
   E_L (cm^{-1}), E_U(cm^{-1}), E_L (K), E_U(K)

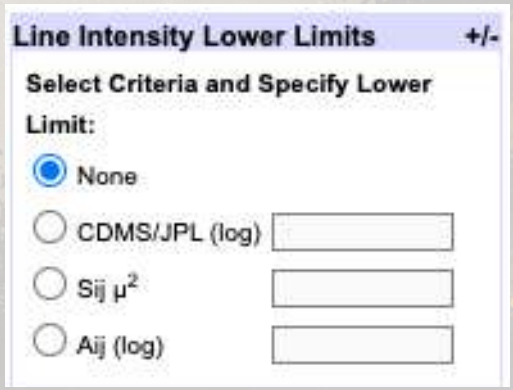
4. Line Intensity Lower limits
   Sij μ^2, Aij (log)

   (μ = electric dipol moment)



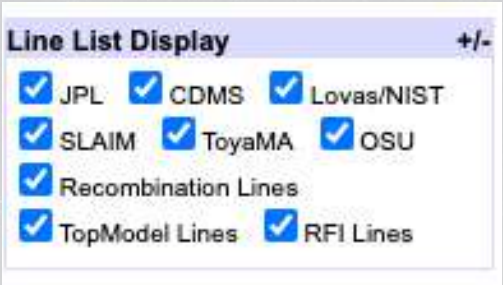


$$E_k = \frac{hc}{k} E_{cm^{-1}} = 1.4387 E_{cm^{-1}}$$



NRAO – Splatalogue: Advanced

Line List Display:

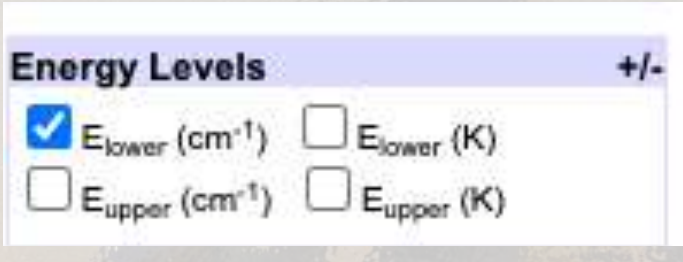


1. Select database:
   JPL, CDMS, Lovas, Recombination lines ….

2. Line strength display:
   Sij μ^2, Sij, Aij

(μ is the dipole moment, useful to estimate Aij)

3. Specify Energy levels:
   E_L (cm^{-1}), E_U(cm^{-1}), E_L (K), E_U(K)



1a. Molecular spectroscopy

NRAO – Splatalogue: Advanced

Search: Molecule: CS, Frequency: 80 to 270 GHz, log(Aij) > -5
Display: CDMS database, Sij μ^2, Sij, Aij, E_L (K), E_U(K)

Found 4 lines, searched 1 frequency ranges, showing 1 - 4
Click on the chemical formula below for more information about that species

	Species	Chemical Name	Freq in GHz (Err) (rest frame, redshifted)	Meas Freq in GHz (Err) (rest frame, redshifted)	Resolved QNs	$S_{ij}\mu^2$ (D^2)	S_{ij}	Log_{10} (A_{ij})	E_L (K)	E_U (K)	Linelist
1	CS v = 0	Carbon Monosulfide		97.98095330 (2.3E-6), 97.98095330	2- 1	7.64426	2.00000	-4.77628	2.35124	7.05355	CDMS
2	CS v = 0	Carbon Monosulfide		146.96902870 (2.6E-6), 146.96902870	3- 2	11.46491	3.00000	-4.21812	7.05356	14.10692	CDMS
3	CS v = 0	Carbon Monosulfide		195.95421090 (1.6E-6), 195.95421090	4- 3	15.28684	4.00000	-3.82753	14.10684	23.51110	CDMS
4	CS v = 0	Carbon Monosulfide		244.93555650 (2.8E-6), 244.93555650	5- 4	19.10860	5.00000	-3.52707	23.51106	35.26605	CDMS

Different colors indicate different ALMA Bands

1a. Molecular spectroscopy

NRAO – Splatalogue: Advanced

Search: Molecule: CH_3OCHO, Frequency: 220 to 221 GHz, $E_U < 200$ K

Display: JPL database, Sij μ^2, Aij, E_L (K), E_U(K)

Found 15 lines, searched 1 frequency ranges, with E_U <= 200 K, showing 1 - 15

Click on the chemical formula below for more information about that species

	Species	Chemical Name	Freq in GHz (Err) (rest frame, redshifted)	Meas Freq in GHz (Err) (rest frame, redshifted)	Resolved QNs	$S_{ij}\mu^2$ (D^2)	Log_{10} (A_{ij})	E_L (K)	E_U (K)	Linelist
1	CH_3OCHO v=0	Methyl Formate		220.16688800 (0.0001), 220.16688800	17(4,13)-16(4,12) E	42.92452	-3.81717	92.58519	103.15148	JPL
2	CH_3OCHO v=0	Methyl Formate		220.19028500 (0.0001), 220.19028500	17(4,13)-16(4,12) A	42.93403	-3.81694	92.57671	103.14411	JPL
3	CH_3OCHO v=0	Methyl Formate	220.70136240 (3.7E-6), 220.70136240		24(1,23)-24(1,24) E	0.81781	-5.68019	158.23362	168.82555	JPL
4	CH_3OCHO v=0	Methyl Formate	220.70151190 (3.7E-6), 220.70151190		24(1,23)-24(0,24) E	1.38023	-5.45289	158.23348	168.82542	JPL
5	CH_3OCHO v=0	Methyl Formate		220.71047000 (5.0E-5), 220.71047000	24(2,23)-24(1,24) E	1.38012	-5.45288	158.23362	168.82599	JPL
6	CH_3OCHO v=0	Methyl Formate		220.71047000 (5.0E-5), 220.71047000	24(2,23)-24(1,24) E	0.81775	-5.68018	158.23348	168.82585	JPL
			220.73579690							

1a. Molecular spectroscopy

NRAO – Splatalogue: Advanced

Search: Molecule: CH_3OCHO, Frequency: 220 to 221 GHz, $E_U < 200$ K

Display: JPL database, Sij μ^2, Aij, E_L (K), E_U(K)

Found 15 lines, searched 1 frequency ranges, with E_U <= 200 K, showing 1 - 15

Click on the chemical formula below for more information about that species

	Species	Chemical Name	Freq in GHz (Err) (rest frame, redshifted)	Meas Freq in GHz (Err) (rest frame, redshifted)	Resolved QNs	$S_{ij}\mu^2$ (D^2)	Log_{10} (A_{ij})	E_L (K)	E_U (K)	Linelist
1	CH_3OCHO v=0	Methyl Formate		220.16688800 (0.0001), 220.16688800	17(4,13)-16(4,12) E	42.92452	-3.81717	92.58519	103.15148	JPL
2	CH_3OCHO v=0	Methyl Formate		220.19028500 (0.0001), 220.19028500	17(4,13)-16(4,12) A	42.93403	-3.81694	92.57671	103.14411	JPL
3	CH_3OCHO v=0	Methyl Formate	220.70136240 (3.7E-6), 220.70136240		24(1,23)-24(1,24) E	0.81781	-5.68019	158.23362	168.82555	JPL
4	CH_3OCHO v=0	Methyl Formate	220.70151190 (3.7E-6), 220.70151190		24(1,23)-24(0,24) E	1.38023	-5.45289	158.23348	168.82542	JPL
5	CH_3OCHO v=0	Methyl Formate		220.71047000 (5.0E-5), 220.71047000	24(2,23)-24(1,24) E	1.38012	-5.45288	158.23362	168.82599	JPL
6	CH_3OCHO v=0	Methyl Formate		220.71047000 (5.0E-5), 220.71047000	24(2,23)-24(1,24) E	0.81775	-5.68018	158.23348	168.82585	JPL
			220.73579690							

1a. Molecular spectroscopy

NRAO – Splatalogu

Search: Molecule

Display: JPL

mate!!

Methyl Formate
CH_3OCHO v=0
Splat ID: 06007

CDMS

line_id	36
species_id	393
ism_hotcore	1
LineList	10
v1_0	1
v2_0	2
linelist	CDMS

JPL

line_id	793
species_id	393
Name	CH3OCHO
Date	April 2009
Contributor	B.J. Drouin
Q_300_0	199602.70
Q_225_0	121102.02
Q_150_0	59072.96
Q_75_00	17548.82
Q_37_50	5772.42
Q_18_75	2030.84
Q_9_375	720.82

Partition function Q(T) at different temperatures

	Species	Chem Nam	E_U (K)	Linelist
1	CH_3OCHO v=0	Methy Forma	03.15148	JPL
2	CH_3OCHO v=0	Methy Forma	03.14411	JPL
3	CH_3OCHO v=0	Methy Forma	68.82555	JPL
4	CH_3OCHO v=0	Methy Forma	68.82542	JPL
5	CH_3OCHO v=0	Methy Forma	68.82599	JPL
6	CH_3OCHO v=0	Methy Forma	68.82585	JPL

NRAO – Splatalogue: Advanced

Miscellaneous +/-

- [ ] No HFS Display
- [ ] Display HFS Intensity
- [ ] Display Unresolved Quantum Numbers
- [ ] Display Upper State Degeneracy
- [ ] Display Molecule Tag
- [x] Display Quantum Number Code
- [ ] Display Lab Ref
- [ ] Display Ordered Frequency ONLY
- [ ] Display NRAO Recommended Frequencies
- [ ] Display Unique Species Tag
- [ ] Display unique line ID #

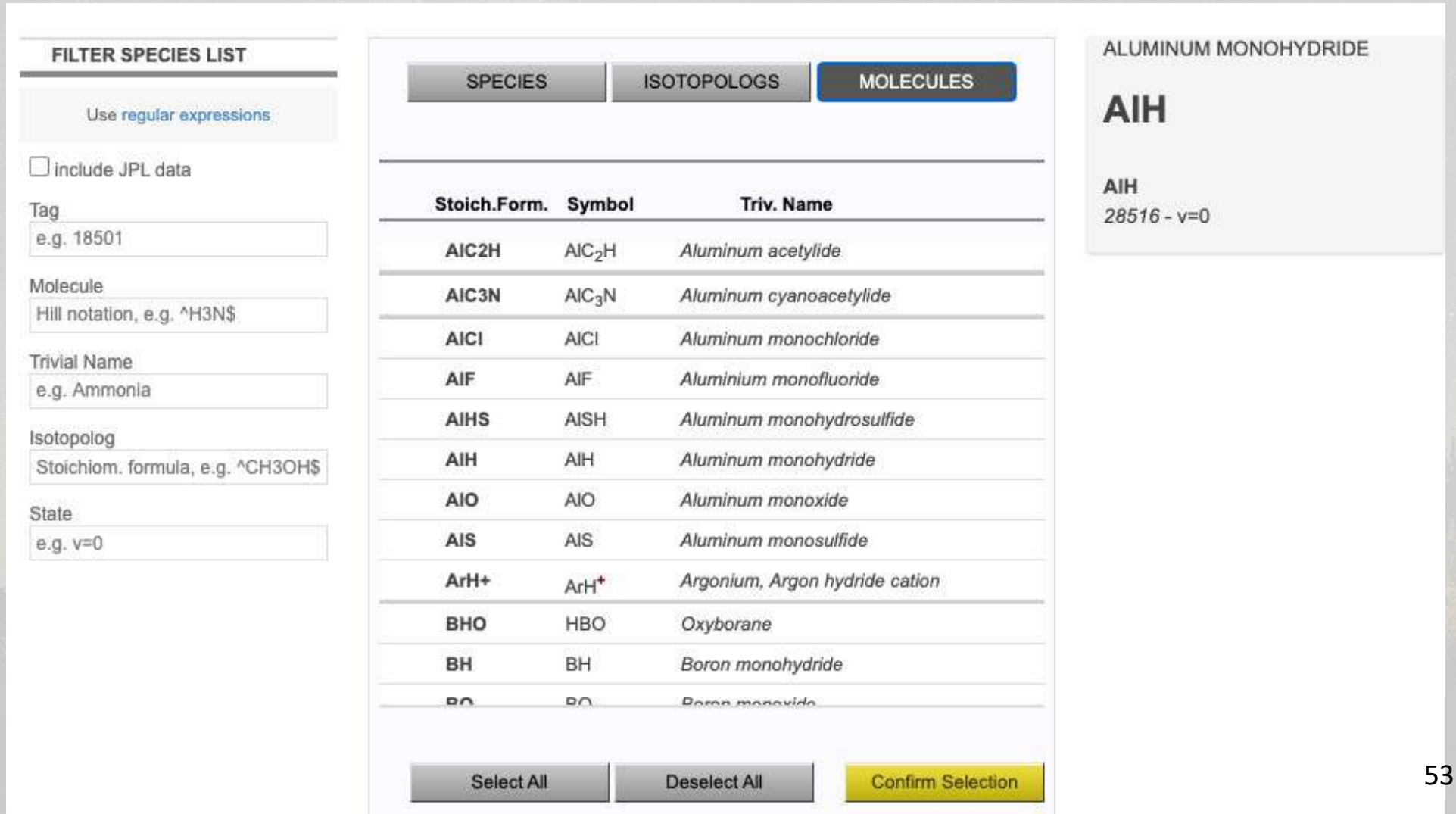
⇒ a code for different quantum numbers

Code Number	Molecular Examples	Electronic State(s)	Unresolved QN	Description and Notes
101	CO, HCN, N_2O	^{1}&Sigma	**N**	N = J, integer values
102	SO, C_2S	^{3}&Sigma	**N J**	N, J, integer values
112	AlF, $C^{17}O$	^{1}&Sigma	**J F+½**	one nuclear spin, I=$^5/_2$ (Al, O)
113	^{33}SO	^{3}&Sigma	**N J F+½**	one nuclear spin, I=$^3/_2$ (Cl)
114	HCCN	^{3}&Sigma	**N J F_1 F+½**	two nuclear spins, I=1 (N and H)
123	AlCl	^{1}&Sigma	**J F+½ F**	two nuclear spins, I=$^5/_2$(Al) I=$^3/_2$(Cl)
	$C^{15}N$, C_2H	^{2}&Sigma	**N J+½ F**	one nuclear spin, I=$^1/_2$(^{15}N, H)
133	SiN, MgNC	^{2}&Sigma	**N J+½ F+½**	one nuclear spin, I=1(N)
144	^{13}CN	^{2}&Sigma	**N J+½ F_1 F**	CDMS: **J**=N+S, **F_1**=J+I(^{13}C), **F**=F_1+I (N)
			N J+½ F_2 F	JPL: **J**=N ± S; **F_1**=S-I (^{13}C)=0, **F_2**=N **F_1**=S+I(^{13}C)=1, **F_2**=N, N ± 1
				(Q=12+2 = 14, for two I=1/2 spins, one I=1)
154	$^{13}C_2H$, $^{13}CCCCH$	^{2}&Sigma	**N J+½ F_1 F+½**	Q=12, 3 spins of 1/2 (I=1/2, I=1/2, S=1/2), N+½=J, J+½=F_1, F_1+½=F
202	$CH_3C^{15}N$, CH_3NC	$^1A_1$	**N K**	no hyperfine structure from nitrogen

1a. Molecular spectroscopy

[CDMS – Cologne Database for Molecular Spectroscopy]

Catalog with several Species, Isotopologues, Molecules



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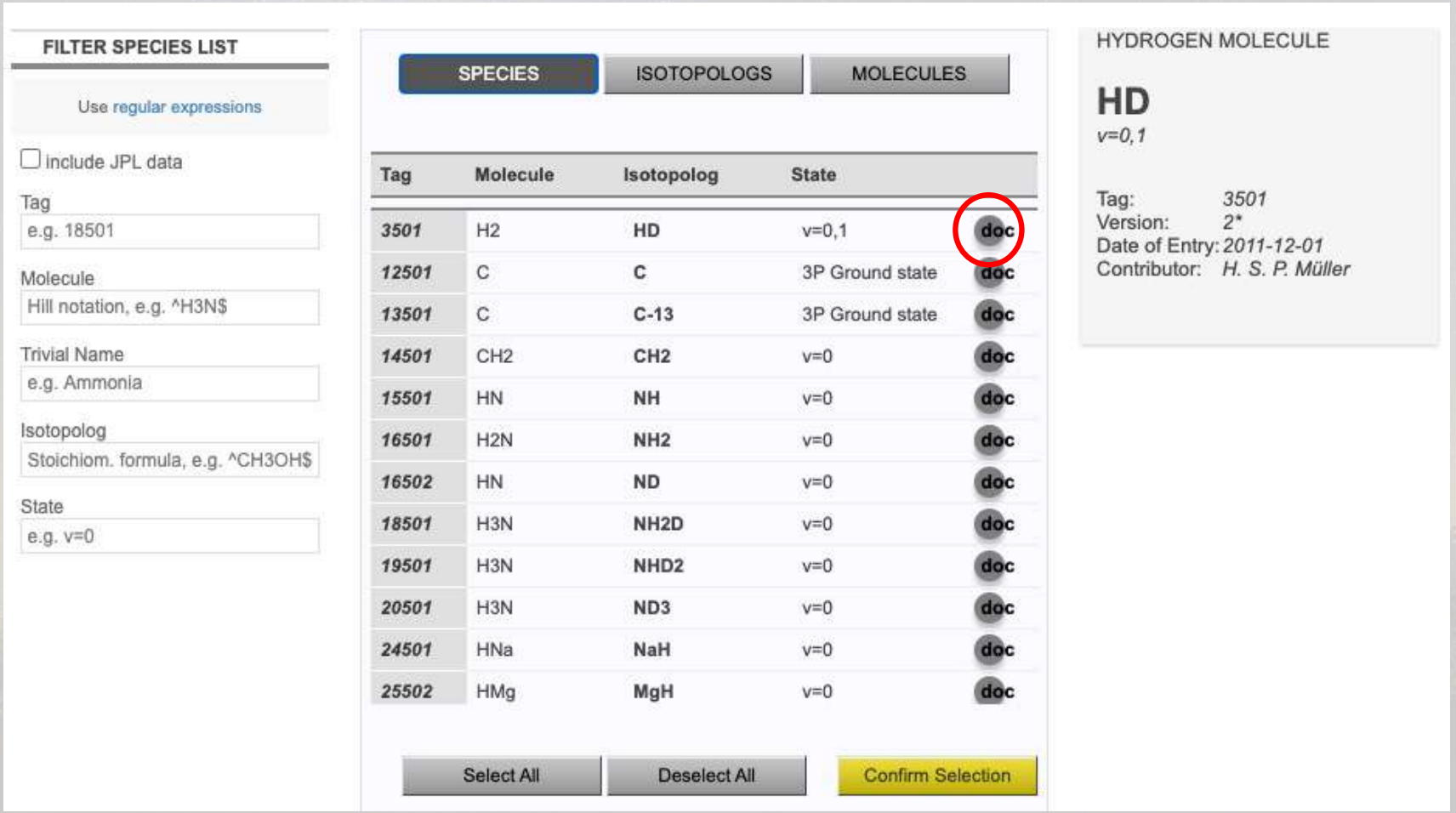

1a. Molecular spectroscopy

HYDROGEN MOLECULE

HD

v=0,1

Tag: *3501*
Version: *2**
Date of Entry: *Dec. 1, 2011*
Contributor: *H. S. P. Müller*

NAVIGATION

- Description
- Molecular Constants
- Partition functions
- Data
- Files
- References
- Stick Spectrum
- Energy Level Plot
- Other databases
- NIST - Lookup
- ChemSpider - Lookup
- Archive

DESCRIPTION

The initial value for the *J"* = 0 transition, employed in the first entry from Sep. 2005 turned out to be off by almost 4 &sigma or almost 600 kHz. The new, more accurate value was measured by
(1) B. J. Drouin, S. Yu, J. C. Pearson, and H. Gupta, 2011, *J. Mol. Struct.*, **1006**, 2.
The *J"* = 1 - 3 transitions were reported by
(2) L. Ulivi, P. de Natale, and M. Inguscio, 1991, *Astrophys. J.*, **378**, L29.
The *J"* = 6 transition was taken from
(3) P. Essenwanger and H. P. Gush, 1984, *Can. J. Phys.*, **62**, 1680.
Infrared transitions were reported by
(4) N. H. Rich, J. W. C. Johns, and A. R. W. McKellar, 1982, *J. Mol. Spectrosc.*, **95**, 432.
The *P*(3) transition was omitted from the final fit.
Predictions should be viewed with caution above *J"* = 8 in the ground vibrational state. The excited state predictions should be viewed with caution throughout because pressure shifts of a few tens of megahertz in the infrared transitions may have a non-negligible effect.
The new *ab initio* dipole moment and its first rotational correction have been derived from
(5) K. Pachuki and J. Komasa, 2008, *Phys. Rev. A*, **78**, Art. No. 052503.
The rotationless value is in very good agreement with experimental determinations employing intensity measurements as well as other theoretical values. The older value of 0.000585 D is definitively incompatible with these numbers. The experimental determinations are hampered by large pressure shifts as well as by high pressure effects on the intensities. The vibrational correction on the dipole moment seems to be small and has been neglected in the present calcultions.
The partition function takes into account both vibrational states; non-negligible individual contributions are given in parentheses.

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1a. Molecular spectroscopy

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Version: *2**

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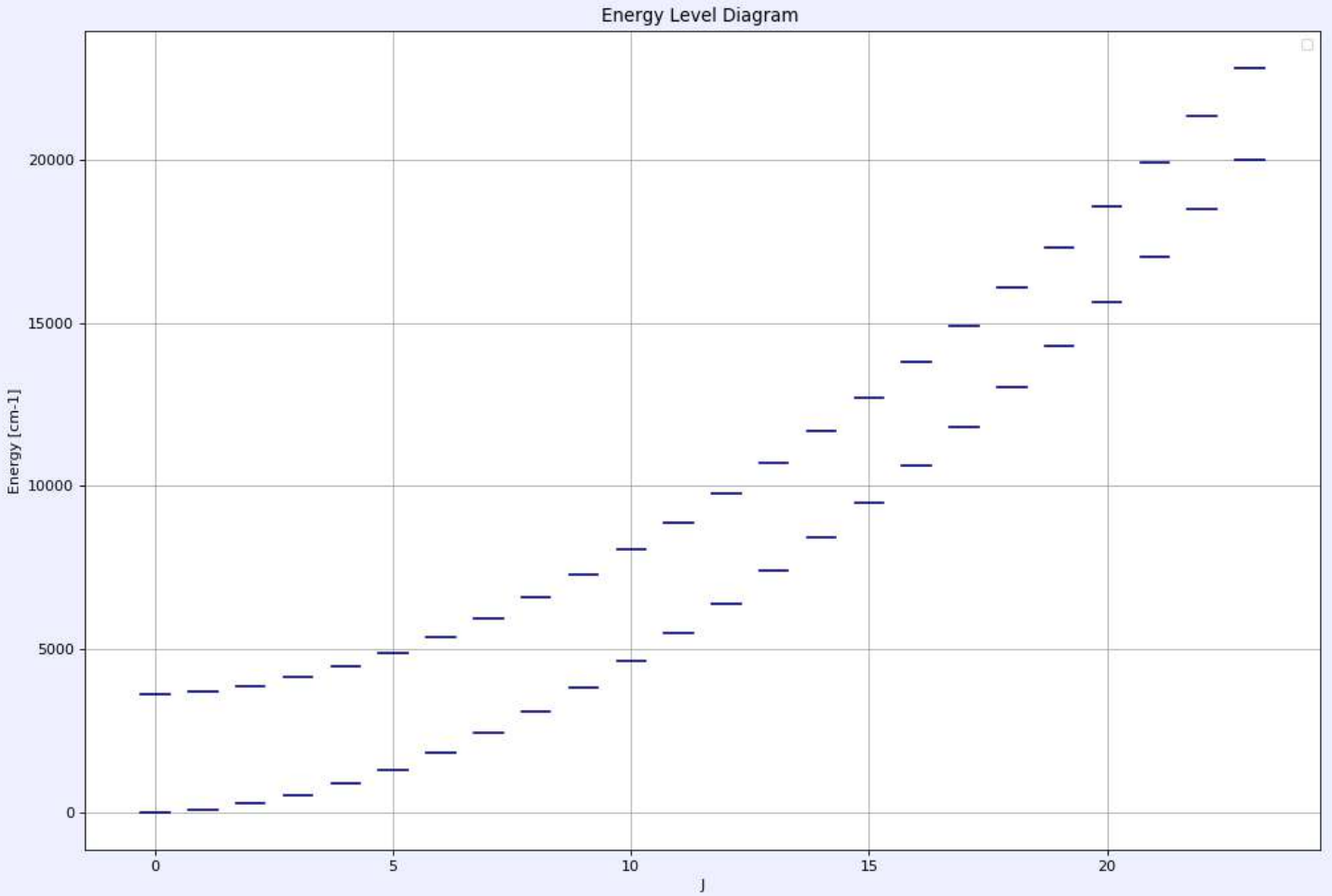

1a. Molecular spectroscopy

CDMS – Cologne Database for Molecular Spectroscopy

A-ALANINE, A-AMINOPROPANE ACID, A-AMINOPROPIONIC ACID

CH3CHNH2COOH

v=0

Tag: *89502*
Version: *1**
Date of Entry: *Oct. 1, 2008*
Contributor: *H. S. P. Müller*

NAVIGATION

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ENERGY LEVEL PLOT