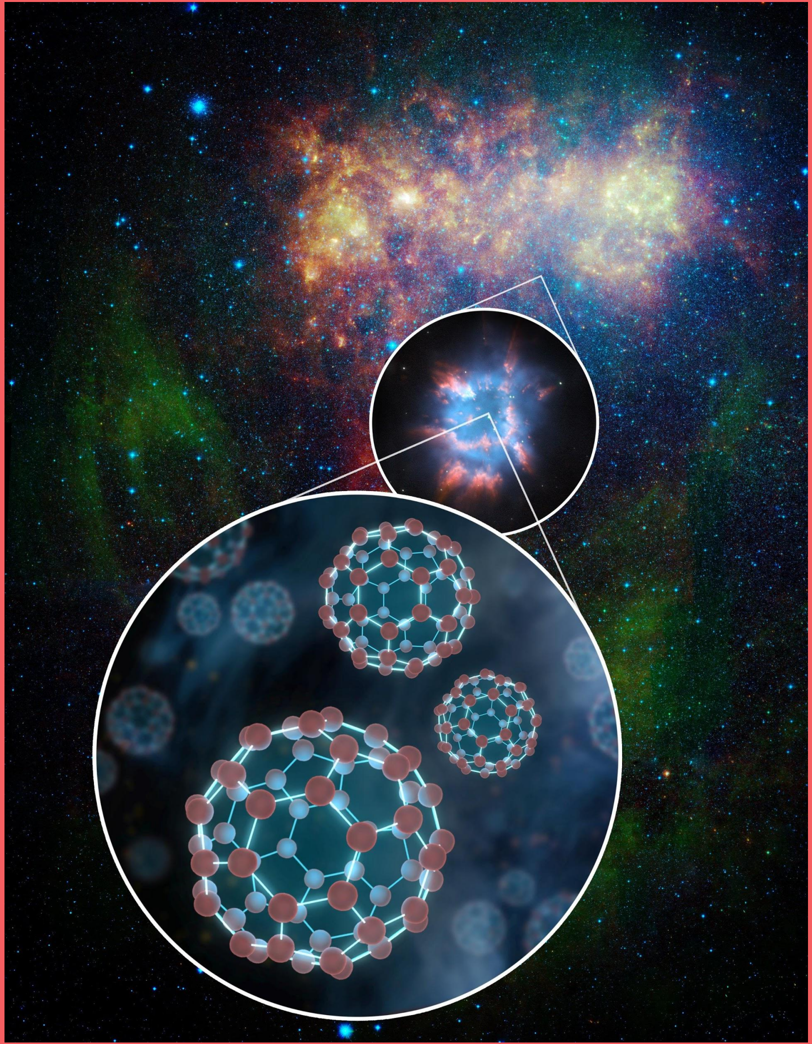
Astroquímica e as moléculas prebióticas no Universo

Dr. Carla Canelo

Ciclo de seminários sobre Astrobiologia (UFES/UFOP) - 04/08/2021

Summary

- Astrochemistry
- Cosmic chemical complexity
- Molecules in Space
- Aromatic molecules in the MIR
- The hot core G331.512-0.103
- Final remarks



Astrochemistry

The study of molecular processes in space.

- Types of chemical reactions in space
- Which reactions occur under which conditions
- Chemical composition of astrophysical objects
- to infer the physical properties
- Links to Astrobiology

A multi-field approach

Observations

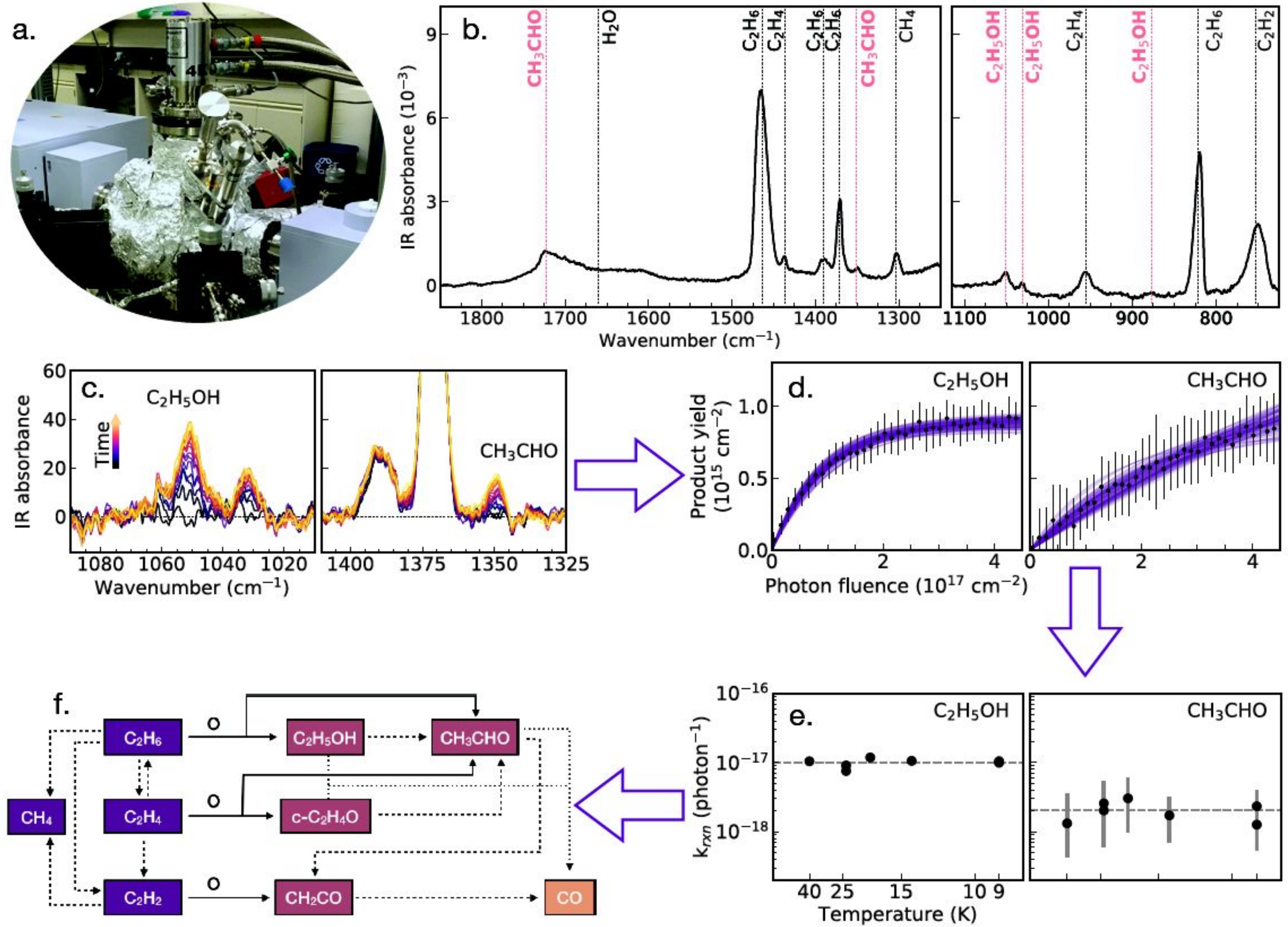
- infrared
- radio
- visual / UV
- X-rays

Models

- early universe
- interstellar clouds
- star-forming regions
- planetary atmospheres

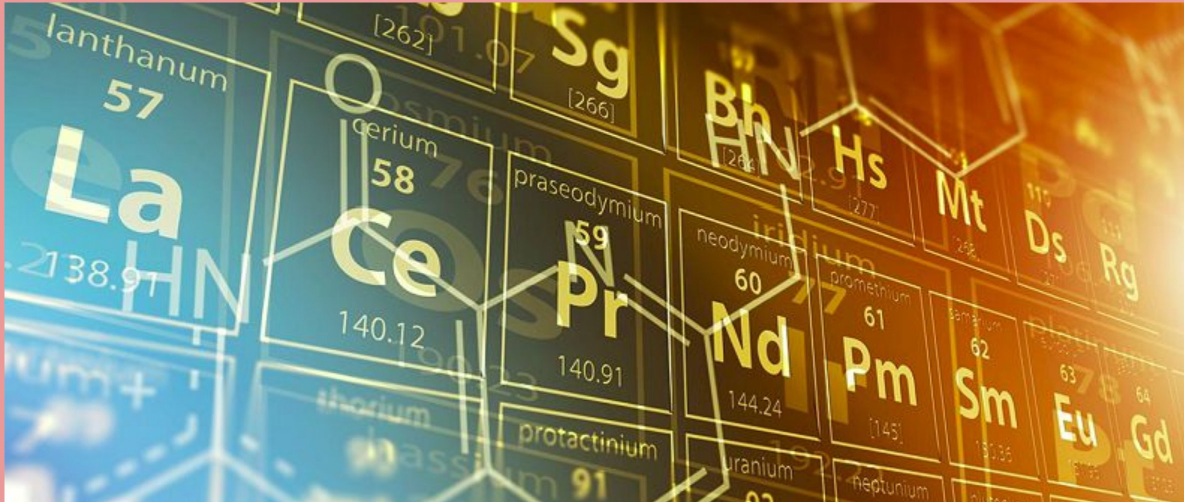
Laboratory / computation

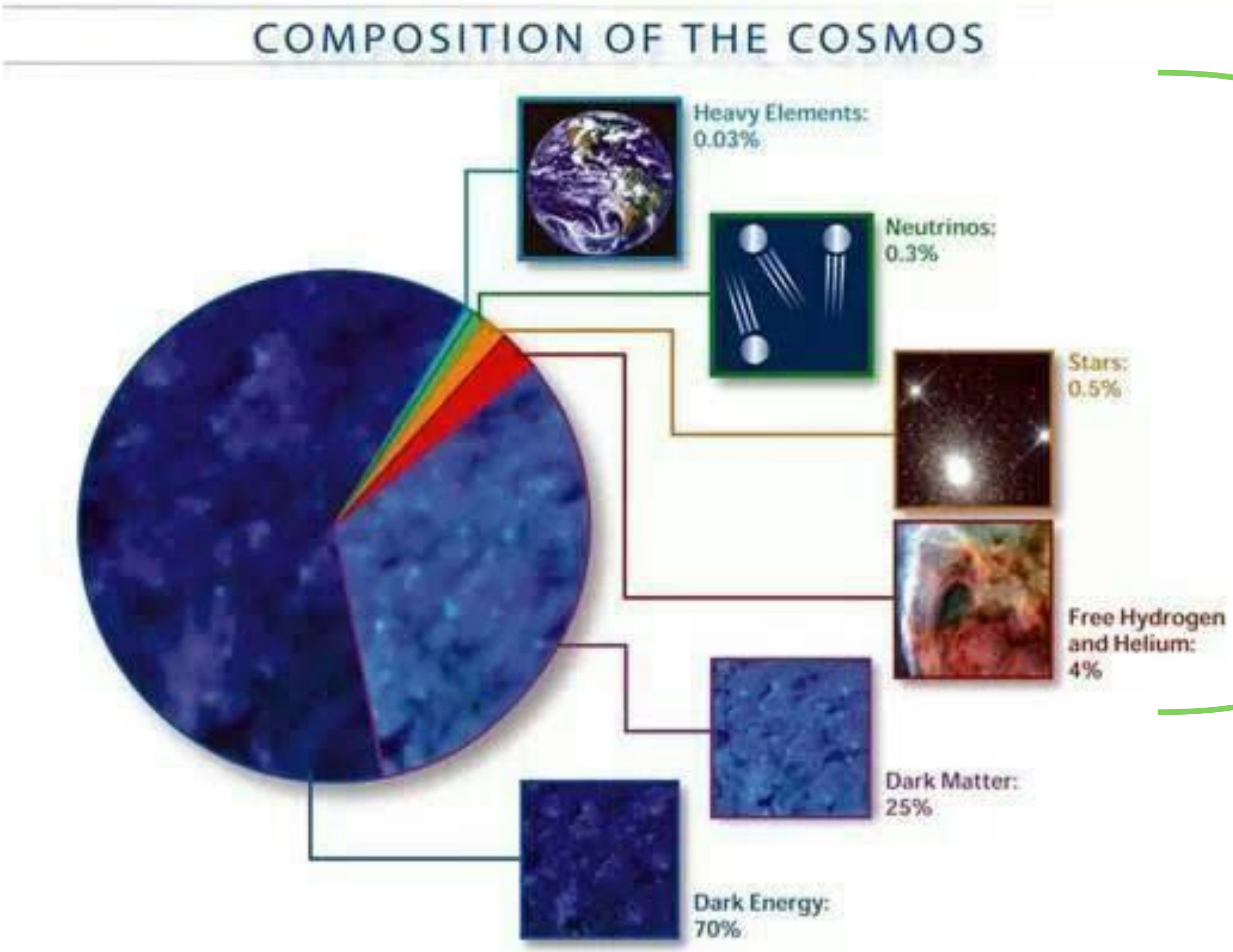
- spectroscopy
- collision rates
- reaction rates
- grain surface processes



(Öberg & Bergin, 2020)

Cosmic chemical complexity





Baryonic matter 5%

Periodic Table

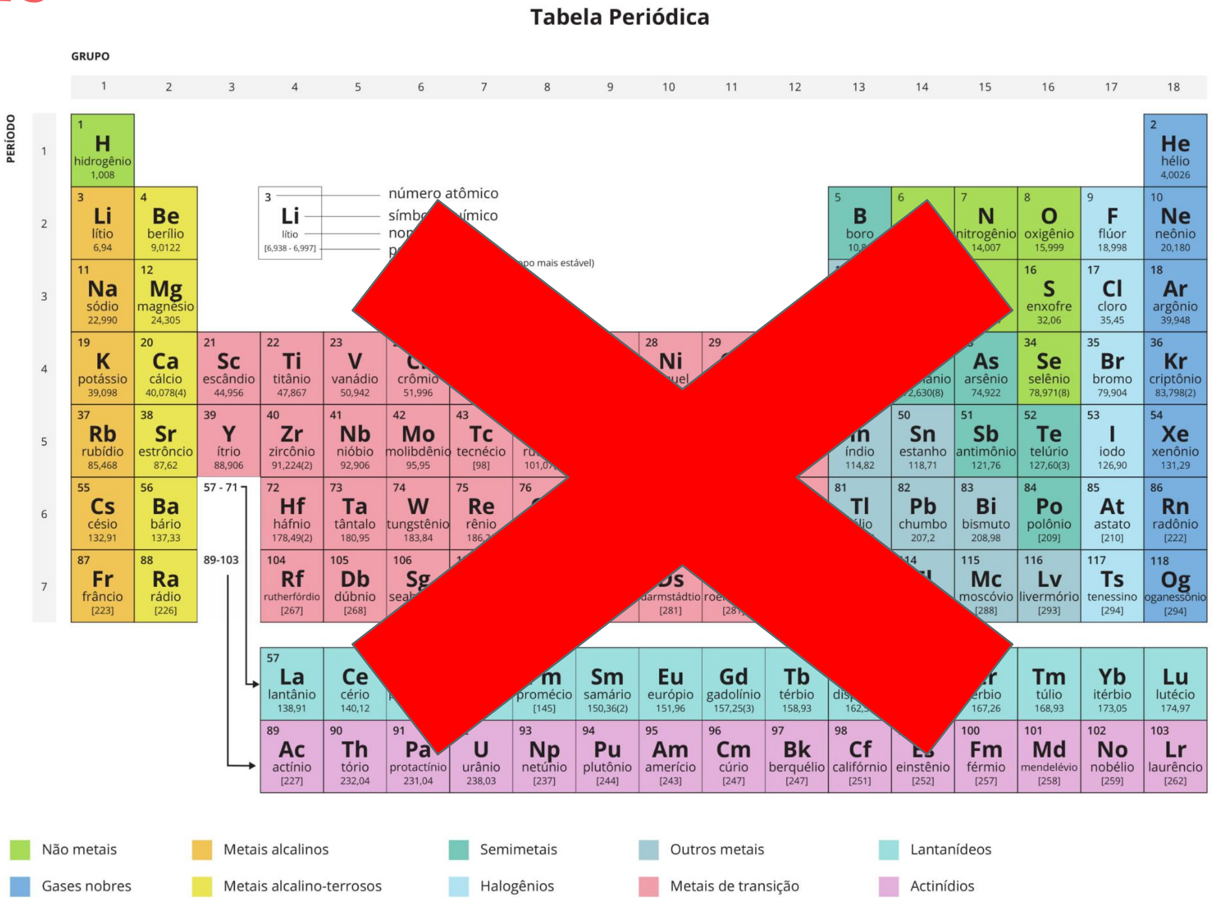
Tabela Periódica

Legenda: 3 — número atômico; Li — símbolo químico; lítio — nome; [6,938 - 6,997] — peso atômico (ou número de massa do isótopo mais estável)

PERÍODO / GRUPO	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** hidrogênio 1,008																	2 **He** hélio 4,0026
2	3 **Li** lítio 6,94	4 **Be** berílio 9,0122											5 **B** boro 10,81	6 **C** carbono 12,011	7 **N** nitrogênio 14,007	8 **O** oxigênio 15,999	9 **F** flúor 18,998	10 **Ne** neônio 20,180
3	11 **Na** sódio 22,990	12 **Mg** magnésio 24,305											13 **Al** alumínio 26,982	14 **Si** silício 28,085	15 **P** fósforo 30,974	16 **S** enxofre 32,06	17 **Cl** cloro 35,45	18 **Ar** argônio 39,948
4	19 **K** potássio 39,098	20 **Ca** cálcio 40,078(4)	21 **Sc** escândio 44,956	22 **Ti** titânio 47,867	23 **V** vanádio 50,942	24 **Cr** crômio 51,996	25 **Mn** manganês 54,938	26 **Fe** ferro 55,845(2)	27 **Co** cobalto 58,933	28 **Ni** níquel 58,693	29 **Cu** cobre 63,546(3)	30 **Zn** zinco 65,38(2)	31 **Ga** gálio 69,723	32 **Ge** germânio 72,630(8)	33 **As** arsênio 74,922	34 **Se** selênio 78,971(8)	35 **Br** bromo 79,904	36 **Kr** criptônio 83,798(2)
5	37 **Rb** rubídio 85,468	38 **Sr** estrôncio 87,62	39 **Y** ítrio 88,906	40 **Zr** zircônio 91,224(2)	41 **Nb** nióbio 92,906	42 **Mo** molibdênio 95,95	43 **Tc** tecnécio [98]	44 **Ru** rutênio 101,07(2)	45 **Rh** ródio 102,91	46 **Pd** paládio 106,42	47 **Ag** prata 107,87	48 **Cd** cádmio 112,41	49 **In** índio 114,82	50 **Sn** estanho 118,71	51 **Sb** antimônio 121,76	52 **Te** telúrio 127,60(3)	53 **I** iodo 126,90	54 **Xe** xenônio 131,29
6	55 **Cs** césio 132,91	56 **Ba** bário 137,33	57 - 71	72 **Hf** háfnio 178,49(2)	73 **Ta** tântalo 180,95	74 **W** tungstênio 183,84	75 **Re** rênio 186,21	76 **Os** ósmio 190,23(3)	77 **Ir** irídio 192,22	78 **Pt** platina 195,08	79 **Au** ouro 196,97	80 **Hg** mercúrio 200,59	81 **Tl** tálio 204,38	82 **Pb** chumbo 207,2	83 **Bi** bismuto 208,98	84 **Po** polônio [209]	85 **At** astato [210]	86 **Rn** radônio [222]
7	87 **Fr** frâncio [223]	88 **Ra** rádio [226]	89-103	104 **Rf** rutherfórdio [267]	105 **Db** dúbnio [268]	106 **Sg** seabórgio [269]	107 **Bh** bóhrio [270]	108 **Hs** hássio [269]	109 **Mt** meitnério [278]	110 **Ds** darmstádtio [281]	111 **Rg** roentgênio [281]	112 **Cn** copernício [285]	113 **Nh** nihônio [286]	114 **Fl** fleróvio [289]	115 **Mc** moscóvio [288]	116 **Lv** livermório [293]	117 **Ts** tenessino [294]	118 **Og** oganessônio [294]
				57 **La** lantânio 138,91	**Ce** cério 140,12	**Pr** praseodímio 140,91	**Nd** neodímio 144,24	**Pm** promécio [145]	**Sm** samário 150,36(2)	**Eu** európio 151,96	**Gd** gadolínio 157,25(3)	**Tb** térbio 158,93	**Dy** disprósio 162,50	**Ho** hólmio 164,93	**Er** érbio 167,26	**Tm** túlio 168,93	**Yb** itérbio 173,05	**Lu** lutécio 174,97
				89 **Ac** actínio [227]	90 **Th** tório 232,04	91 **Pa** protactínio 231,04	92 **U** urânio 238,03	93 **Np** netúnio [237]	94 **Pu** plutônio [244]	95 **Am** amerício [243]	96 **Cm** cúrio [247]	97 **Bk** berquélio [247]	98 **Cf** califórnio [251]	99 **Es** einstênio [252]	100 **Fm** férmio [257]	101 **Md** mendelévio [258]	102 **No** nobélio [259]	103 **Lr** laurêncio [262]

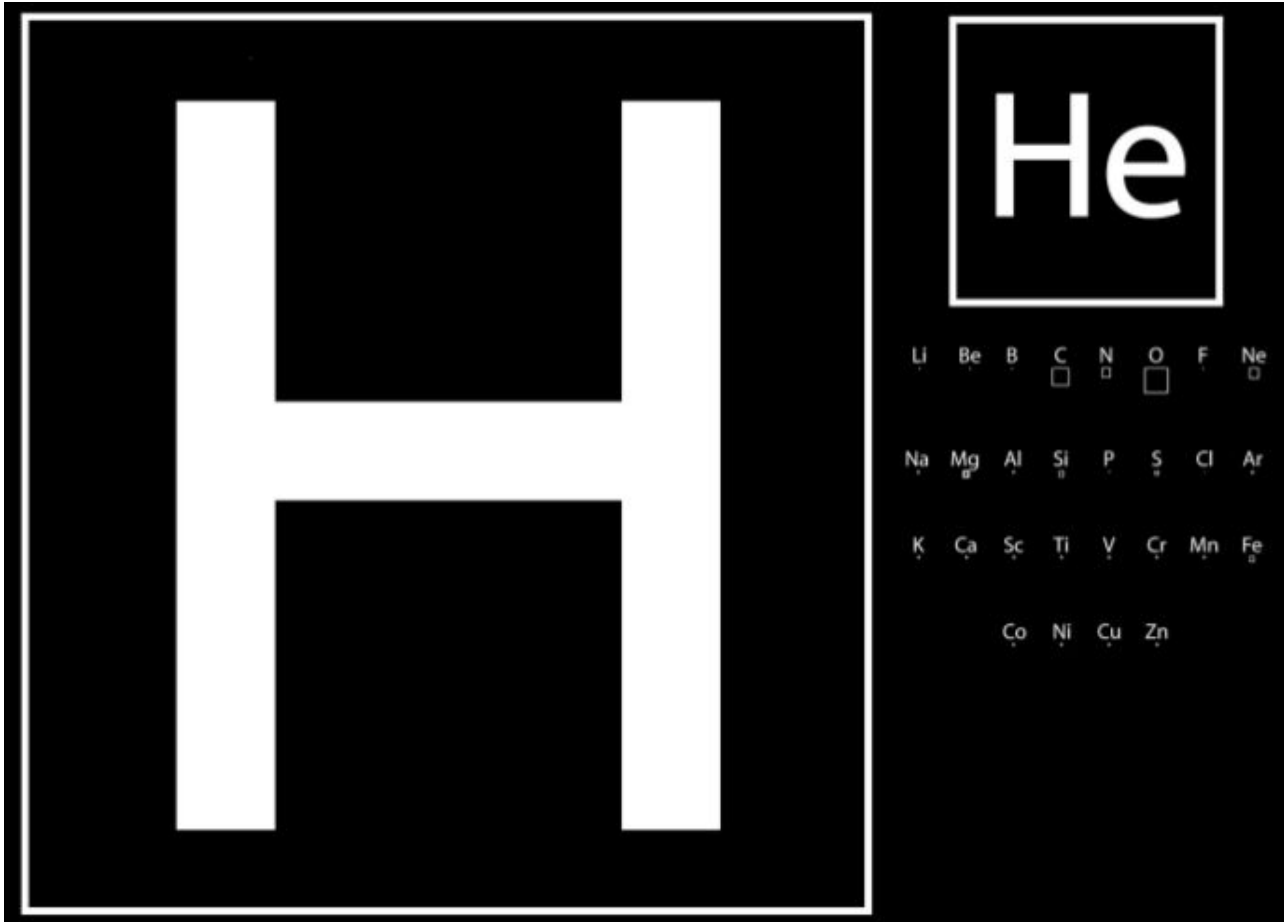
- Não metais
- Gases nobres
- Metais alcalinos
- Metais alcalino-terrosos
- Semimetais
- Halogênios
- Outros metais
- Metais de transição
- Lantanídeos
- Actinídios

Periodic Table

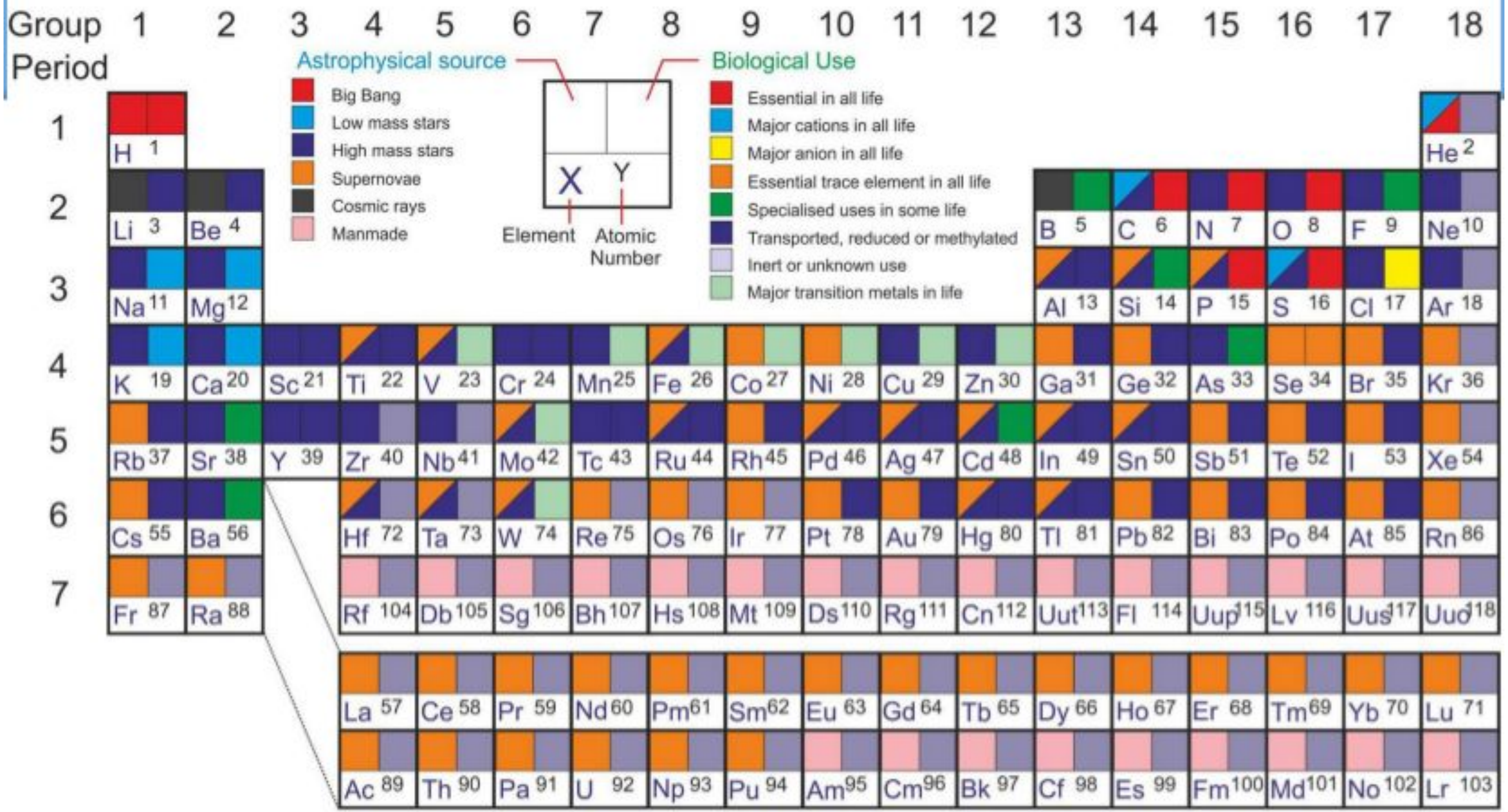


"Astronomers' Periodic Table"

*CHONPS

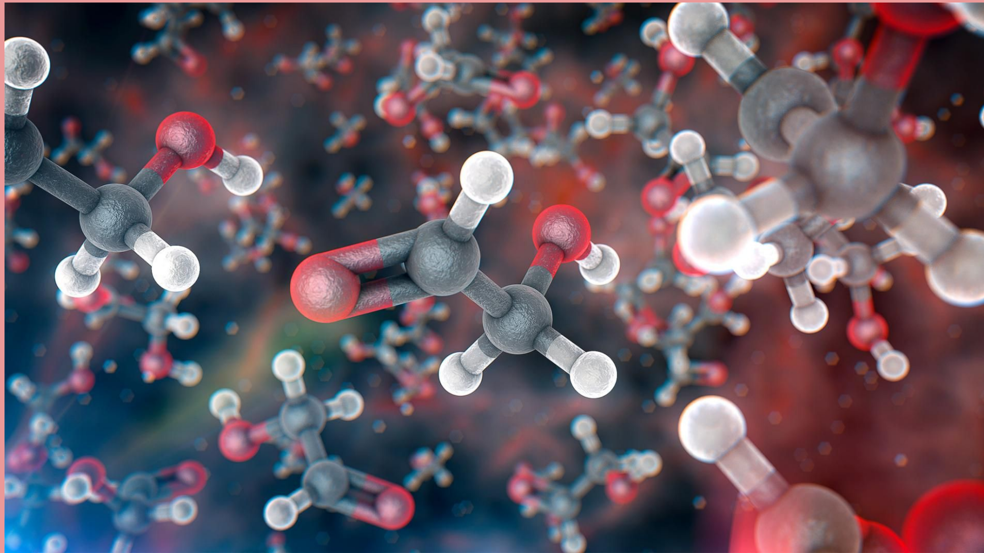


© Charles S Cockell, v. 1.0 [June 2015]: The Astrobiological Periodic Table



Biological data from Wackett, L.P., Dodge, A.G., Ellis, L.B.M. (2004) *Applied and Environmental Microbiology* **70**, 647-655.

Molecules in Space



More than 200 molecules detected in ISM

Molecules in the Interstellar Medium or Circumstellar Shells (as of 08/2020)

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_2	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}^*
AlF	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}^*
AlCl	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}^{+*}
C_2^{**}	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
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	CH_3CHCH_2O	$CH_3C(O)CH_2OH$ (2020)		
CH^+	HCN	$C_2H_2^*$	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3OCH_2OH			
CN	HCO	NH_3	CH_4^*	CH_3SH	c-C_2H_4O	l-HC_6H^*	$CH_3C(O)NH_2$				
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	H_2CCHOH (?)	CH_2CHCHO(?)	C_8H^-				
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6				
CP	HOC^+	HNCO	HCOOH	NH_2CHO	CH_3NCO	H_2NCH_2CN	CH_3CH_2SH(?)				
SiC	H_2O	HNCS	H_2CNH	C_5N	HC_5O	CH_3CHNH	CH_3NHCHO				
HCl	H_2S	$HOCO^+$	H_2C_2O	l-HC_4H^*	$HOCH_2CN$ (2019)	CH_3SiH_3	HC_7O				

to be continued...

Line forests

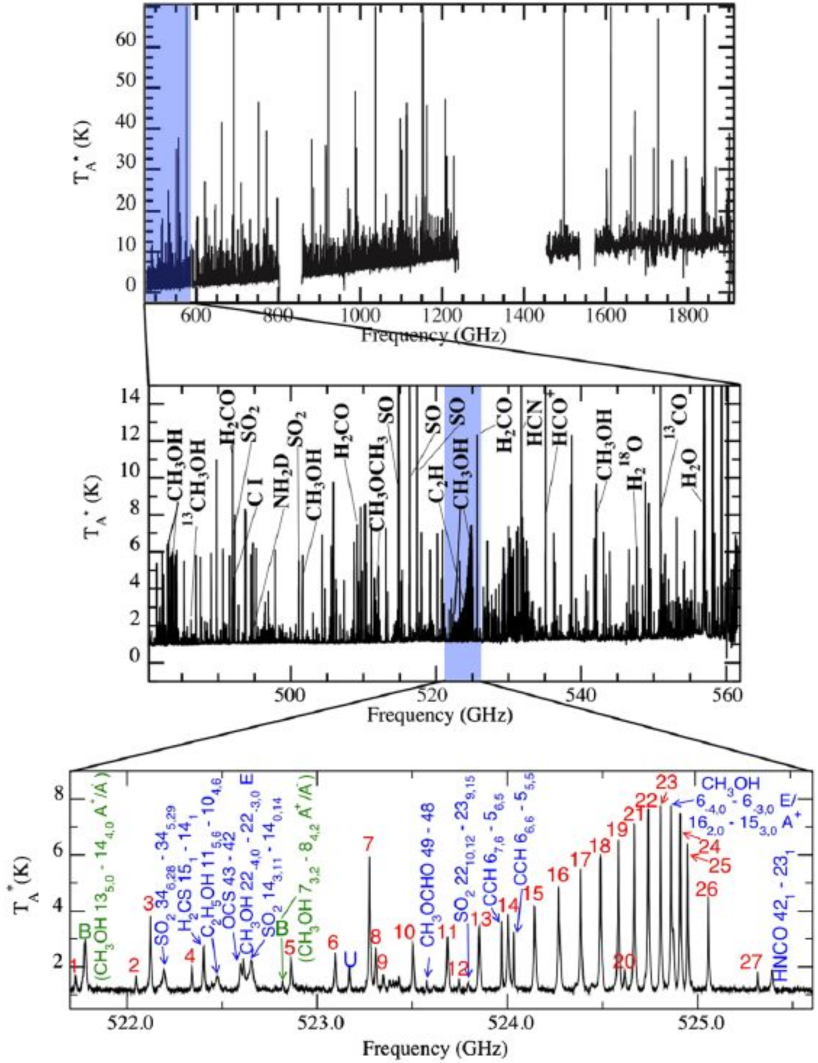


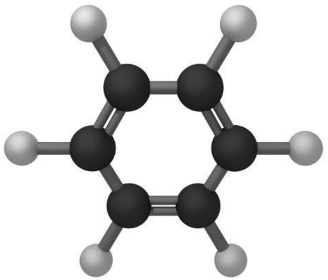
Fig: HIFI spectral survey of the Orion KL region. Top panel: The complete spectral scan (490 GHz to 1.9 THz) reveals the rich line forest. There are some 105 lines in this spectrum. Middle panel: A zoom in on the 490–530 GHz spectral range with some of the stronger lines identified. Bottom panel: The 522:5–525:5 GHz range shows velocity-resolved lines. The numbered lines are CH3OH lines used in the analysis of the temperature structure of the region (Tielens 2013).

COMs - Complex Organic Molecules

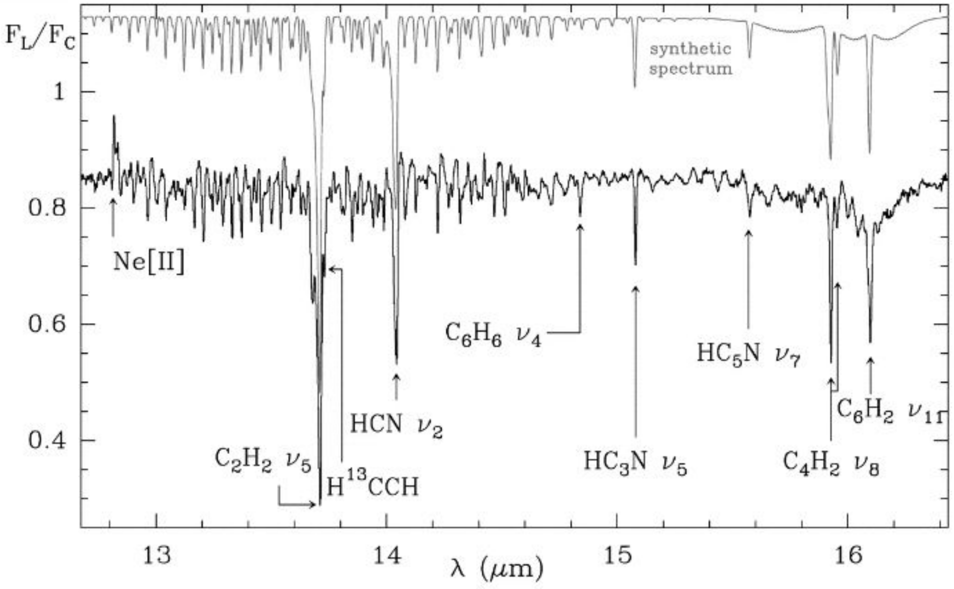
- molecules with 6 or more atoms including C
  (Herbst & van Dishoeck 2009)

- CH_3OH, CH_3CN, CH_3CHO, CH_3OCH_3, ...

- **Prebiotic molecules**
  - NH_2CHO (formamide)
  - Benzene



Cernicharo et al 2001 (ISO)



Search for interstellar emission of N-heterocycles

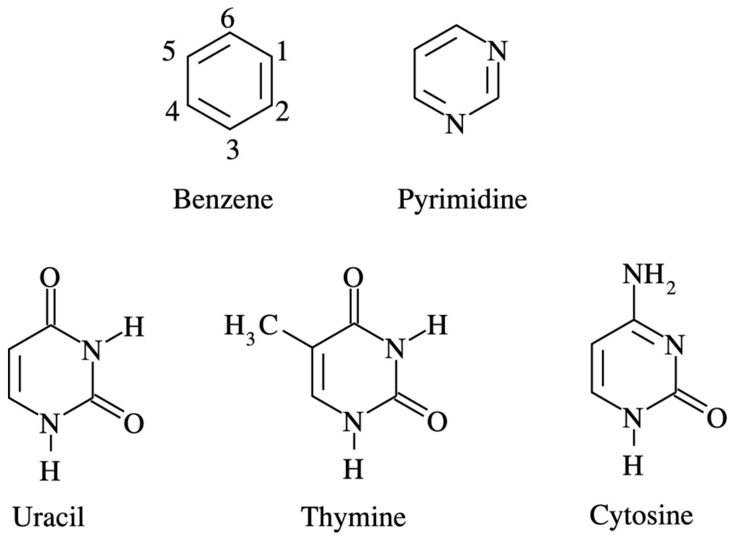


Fig.: Molecular structure of benzene, pyrimidine and pyrimidinic nucleobases uracil, thymine and cytosine (Mendoza et al. 2013).

- Motivation → prebiotic chemistry
- Formation of nucleobases
- Presence in meteorites (e.g. Murchison) (Allamandola et al. 1999, Martins et al. 2005, 2008)
- Large dipole moments → detection at radio wavelengths (Charnley et al. 2005)

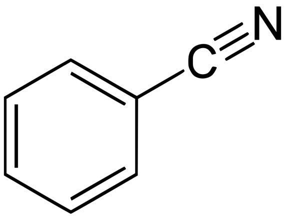
N-heterocycles (tentatives of) detection in ISM

- Vinyl cyanide, pyrimidine and pyridine in 1973
  (Martha Simon & Michal Simon, 1973)

- Pyridine, pyrimidine, quinoline, isoquinoline
  (Charnley et al. 2005, Kuan et al. 2006)

- Benzonitrile!

  (Mcguire et al. 2019)



Still a challenge:

- Low abundances
- Photodissociation

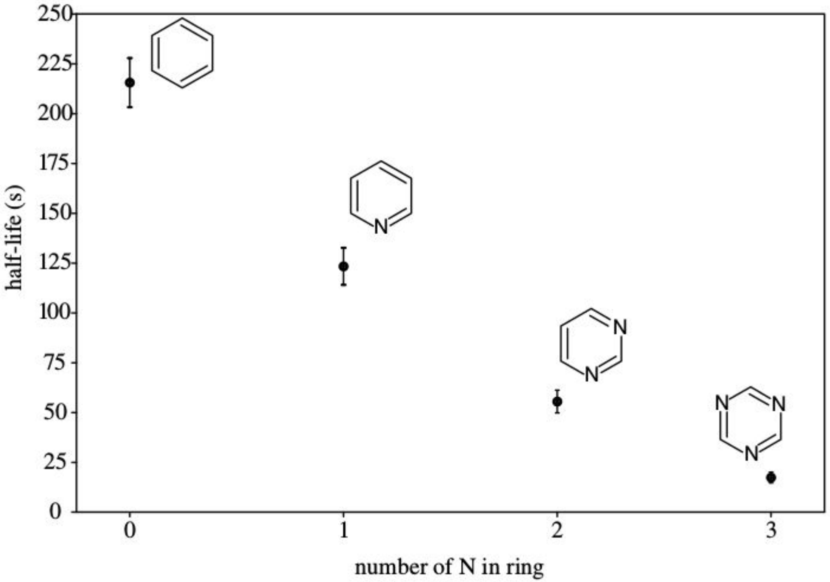
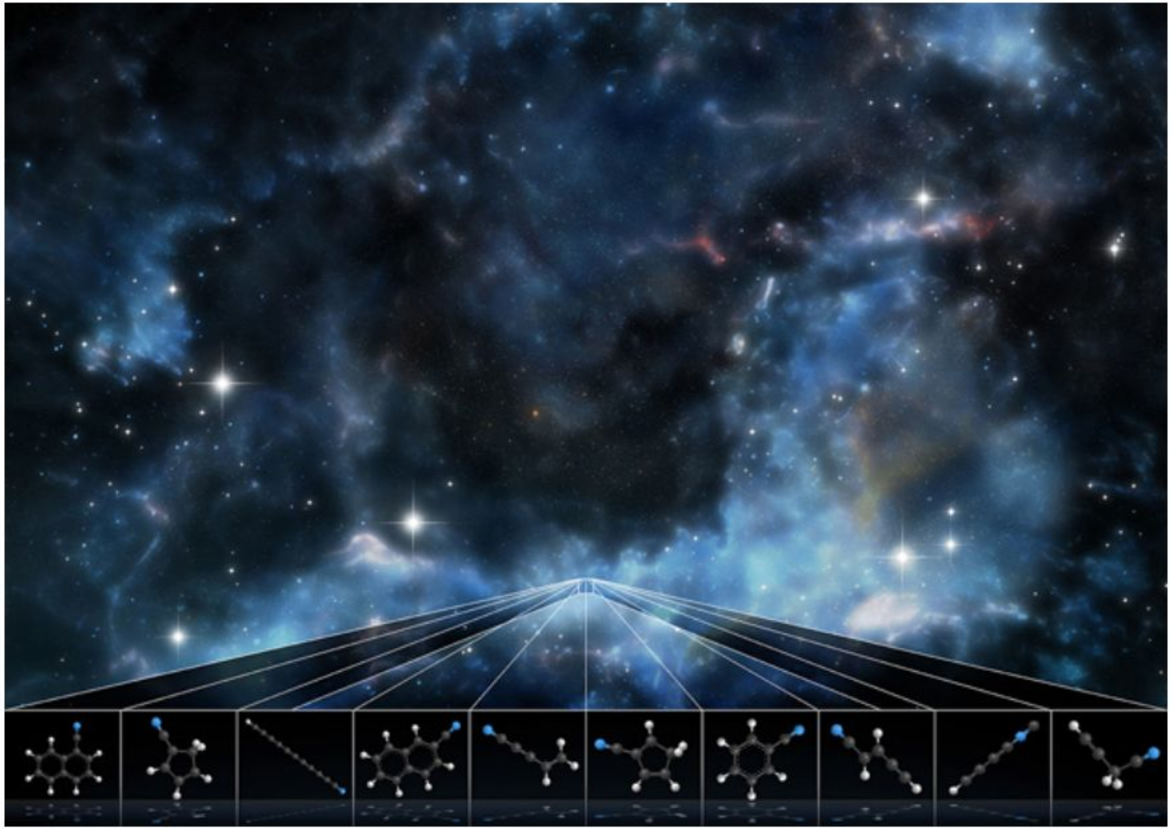


Fig.: The half-lives of the three N-heterocycles plotted against the number of nitrogen atoms in the ring.
(Z. Peeters et al. 2005).

Green Bank Discovers Many Complex Molecules Never Before Seen In Space

Source: Green Bank   Posted March 18, 2021 10:46 PM   0 Comments



Series of 9 papers!!

GOTHAM
Green Bank Telescope Observations of TMC-1: Hunting Aromatic Molecules

http://astrobiology.com/2021/03/geen-bank-discovers-man-complex-molecules-never-before-seen-in-space.html

TMC - 1

- very early evolutionary phase (precollapse)

- source of unsaturated carbon-chain molecules

- **evidence** of five-membered and bicyclic CN-functionalized **rings**

→ **unexplored area of organic chemistry in space**

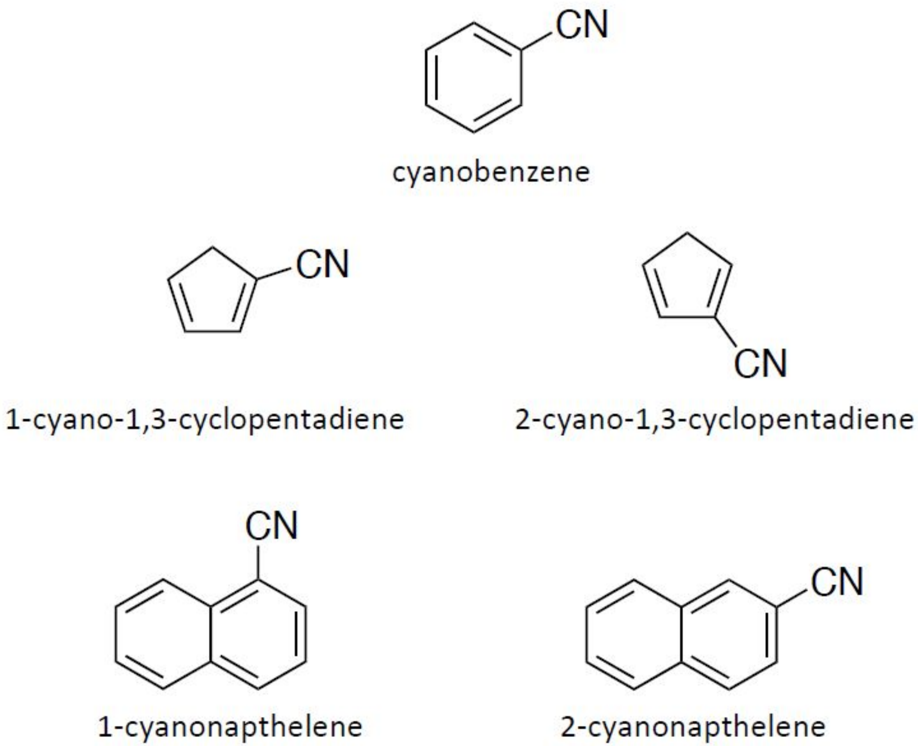
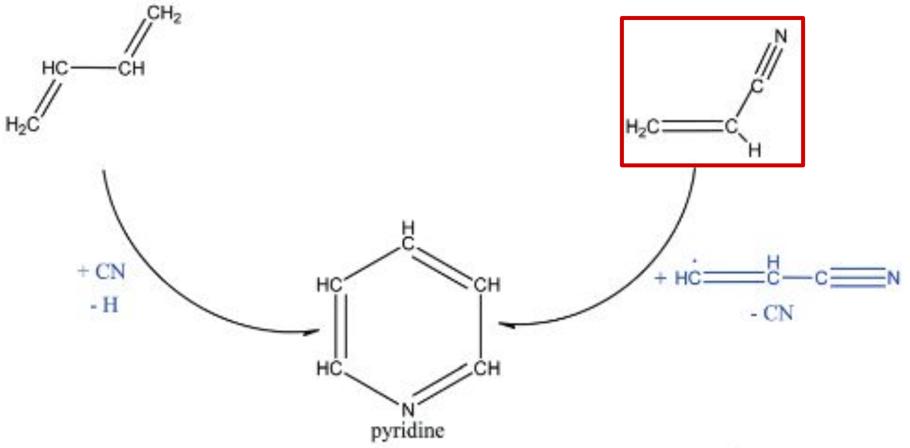


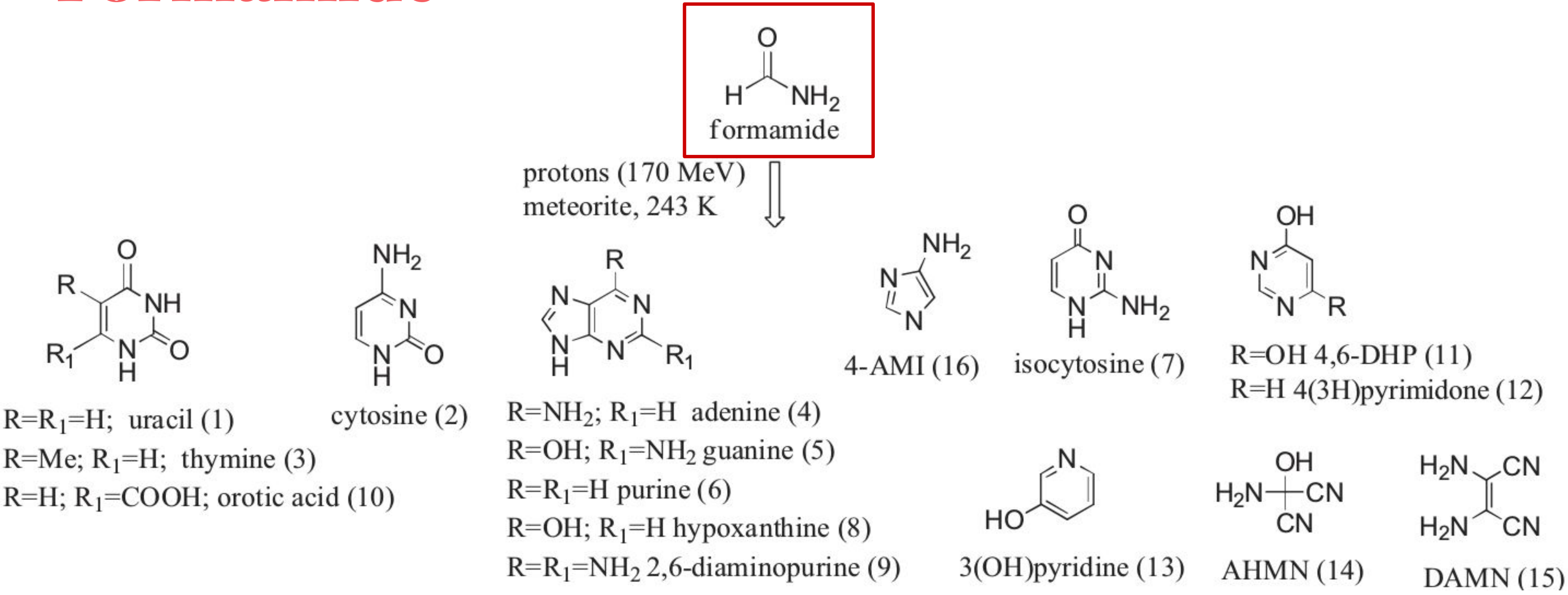
Figure 1: Structures and common chemical names of the five aromatic or cyclic molecules that have recently been discovered in the dark molecular cloud TMC-1 on the basis of precise laboratory rest frequencies using the 100 m Green Bank Telescope.

Search for N-heterocycles precursors

- HNCO, HC3N, C3H and $HC3NH^+$ (Majumdar et al. 2015)
- Formamide
- Vinyl cyanide (C2H3CN) (Parker & Kaiser, 2017)



Formamide



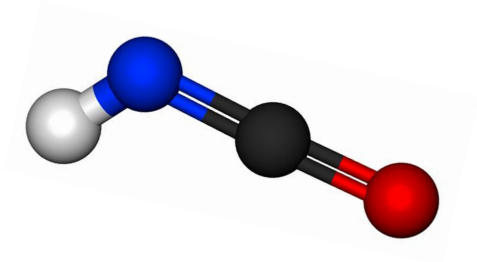
Products of high-energy proton irradiation of formamide in the presence of meteorites. Nucleobases, nucleobase analogs, and intermediates of the condensation (Saladino et al; 2015).

HNCO as a prebiotic molecule

- Contains four of the biogenic elements (CHONPS)

- Can form molecules with peptide bonds in solid state
  - amino acids
  - proteins

(Fedoseev et al. 2015)



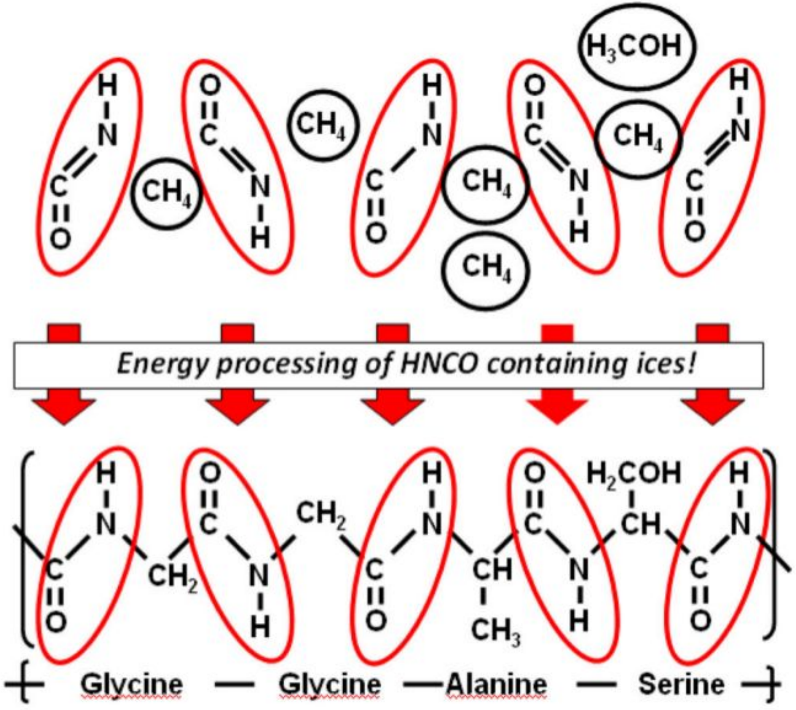


Figure 6. A schematic that illustrates the potential importance of HNCO as a simple bearer of peptide bonds for the production of amino acids in interstellar ices.

Formation of HNCO

- Gas phase reactions do not reproduce the observations

- GRAIN REACTIONS

  Interstellar ice analogues processed by proton or UV radiation

(Fedoseev et al. 2015)

$$NH + CO \rightarrow HNCO$$

$$NH_2 + CO \rightarrow HNCO + H$$

$$N + CO \rightarrow NCO$$

$$H + NCO \rightarrow HNCO$$

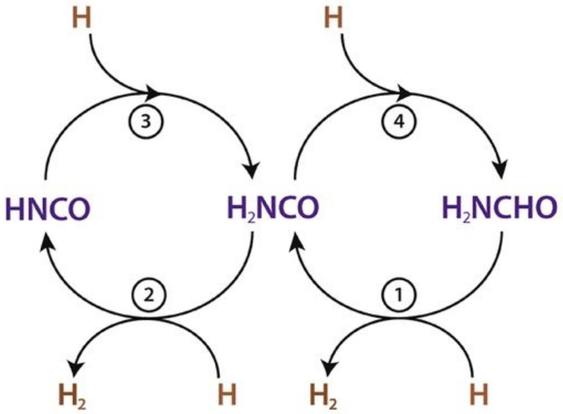
HNCO and NH_2CHO

- [HNCO]/[NH2CHO] ~ 3.0

  (e.g. Mendoza et al. 2014)

- They may share a common solid state formation scheme

  (Haupa et al. 2019)



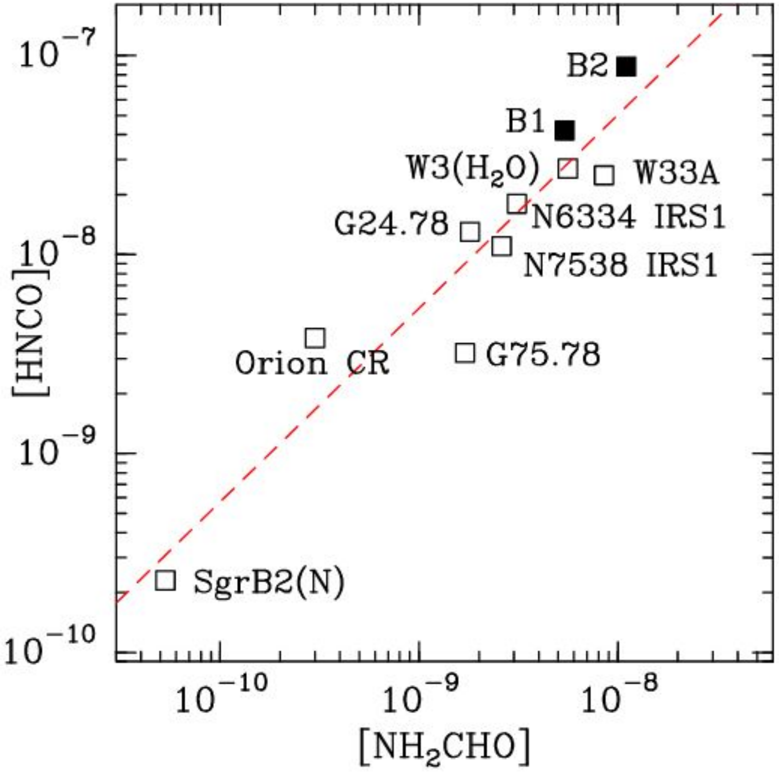
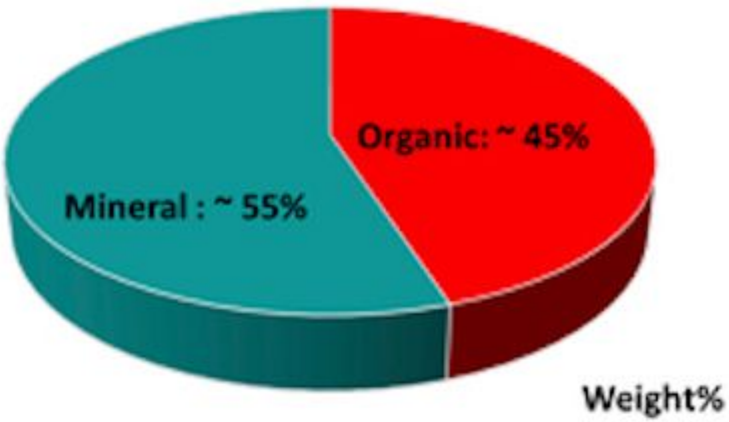


Figure 7. Comparison of molecular abundances for NH_2CHO and HNCO in a sample of Galactic sources. Filled symbols indicate our values measured towards the protostellar shocks B1 and B2. The data were taken from by Jackson, Armstrong & Barrett (1984), Sutton et al. (1995), Bisschop et al. (2007), Martín et al. (2008), and Halfen et al. (2011). The best power-law fit $[HNCO] = 3.0 \times [NH_2CHO]^{0.97}$ is drawn in dashed.

Comets, asteroids and meteorites

67P/Churyumov-Gerasimenko

- Rosetta/Philae mission
- **glycine**



Meteorite Murchison

Rich in organic molecules

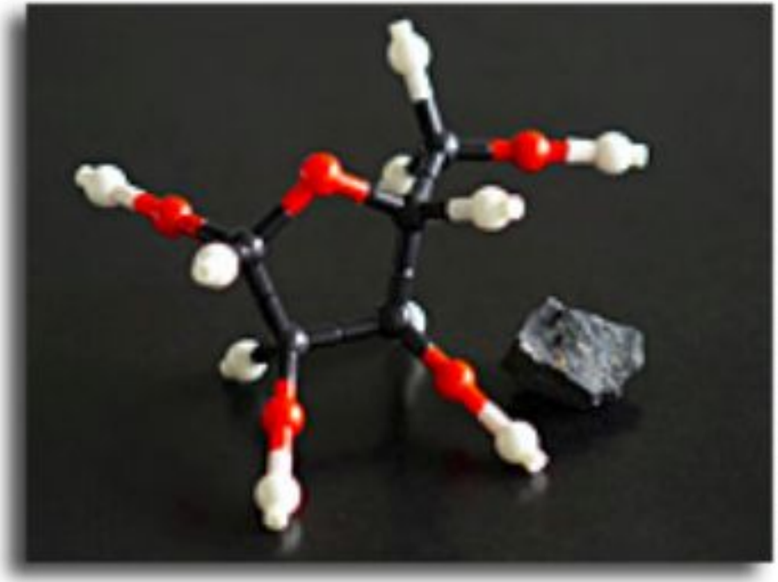
Compound class[14]	Concentration (ppm)
Amino acids	17–60
Aliphatic hydrocarbons	>35
Aromatic hydrocarbons	3319
Fullerenes	>100
Carboxylic acids	>300
Hydrocarboxylic acids	15
Purines and pyrimidines	1.3
Alcohols	11
Sulphonic acids	68
Phosphonic acids	2

Astrobiology Web - 18/11/2019

ASTROCHEMISTRY

First Detection of Sugars in Meteorites Gives Clues to Origin of Life

0

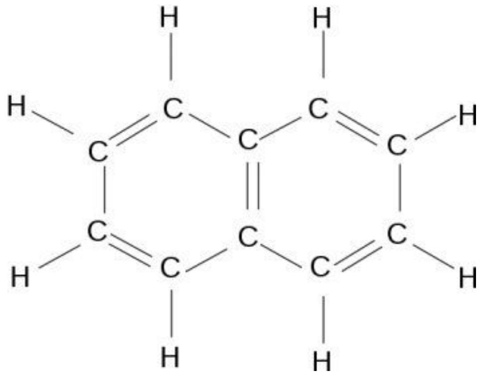


Yoshihiro Furukawa

An international team has found sugars essential to life in meteorites. The new discovery adds to the growing list of biologically important compounds that have been found in meteorites, supporting the hypothesis that chemical reactions in asteroids - the parent bodies of many meteorites - can make some of life's ingredients.

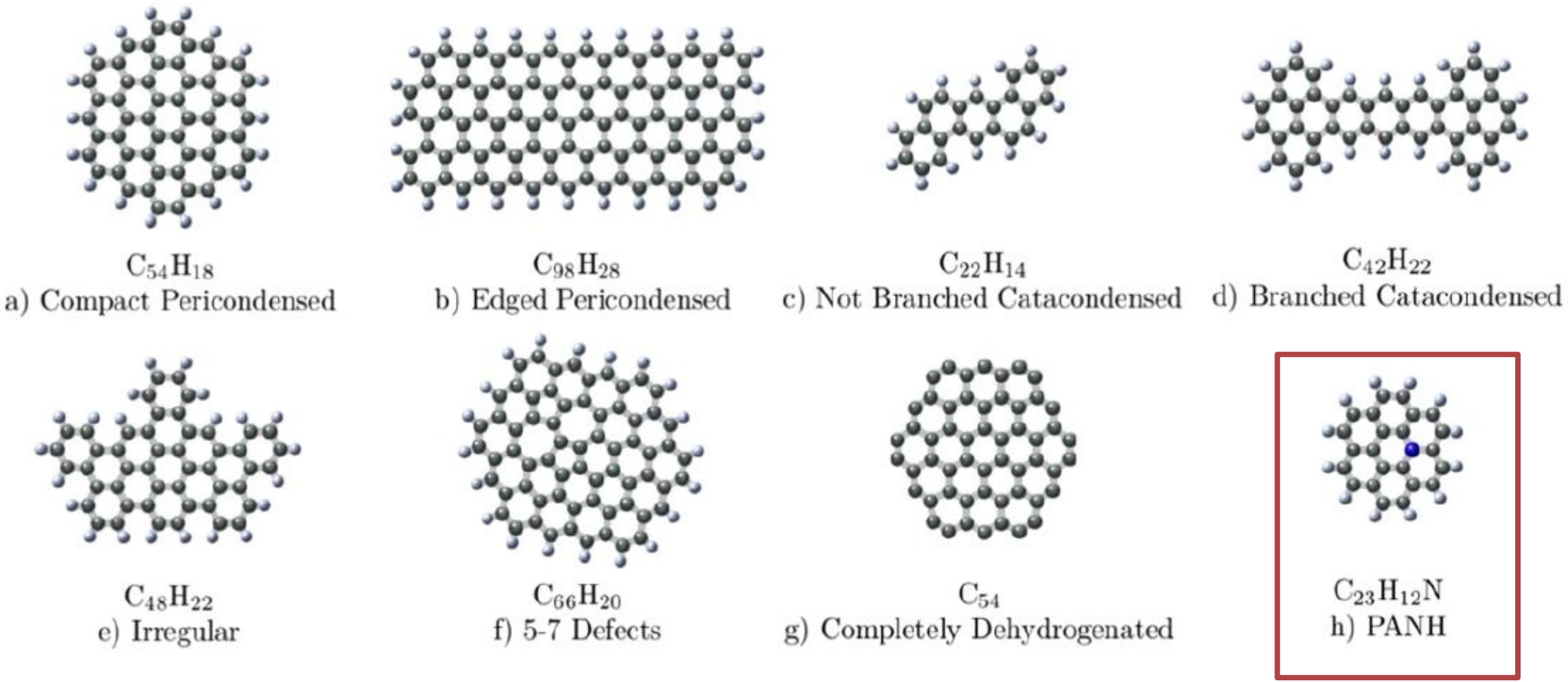
PAHs (Polycyclic aromatic hydrocarbons)

- 15% of the carbon in the interstellar medium (ISM) (Joblin et al. 1992)
- Dominant organic material (Ehrenfreund et al. 2006)
- 50% of the mid-IR luminosity (Li et al. 2004)
- Prebiotic role (PAH World) (Ehrenfreund et al. 2006)



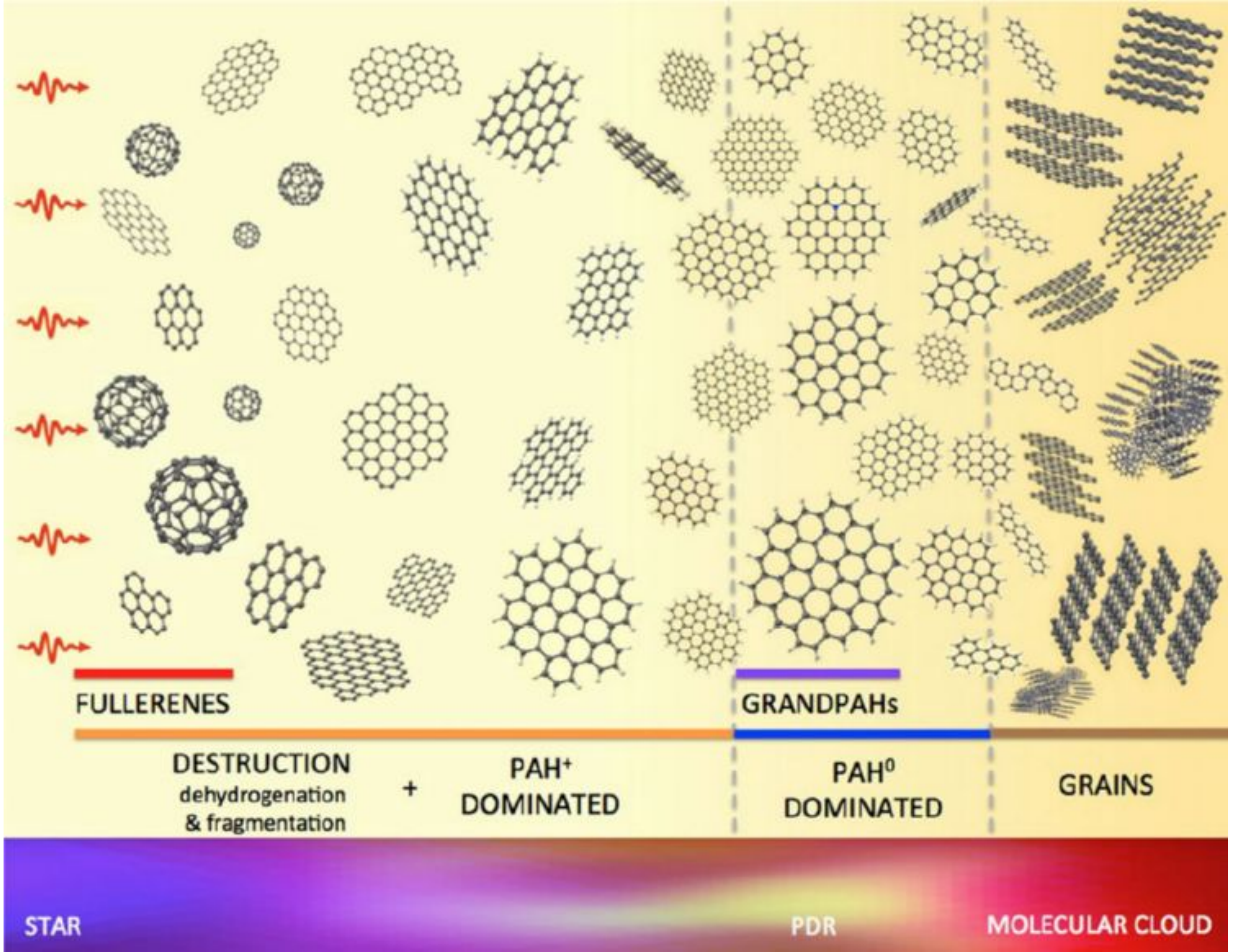
Naphthalene $C_{10}H_8$

Structures of PAHs

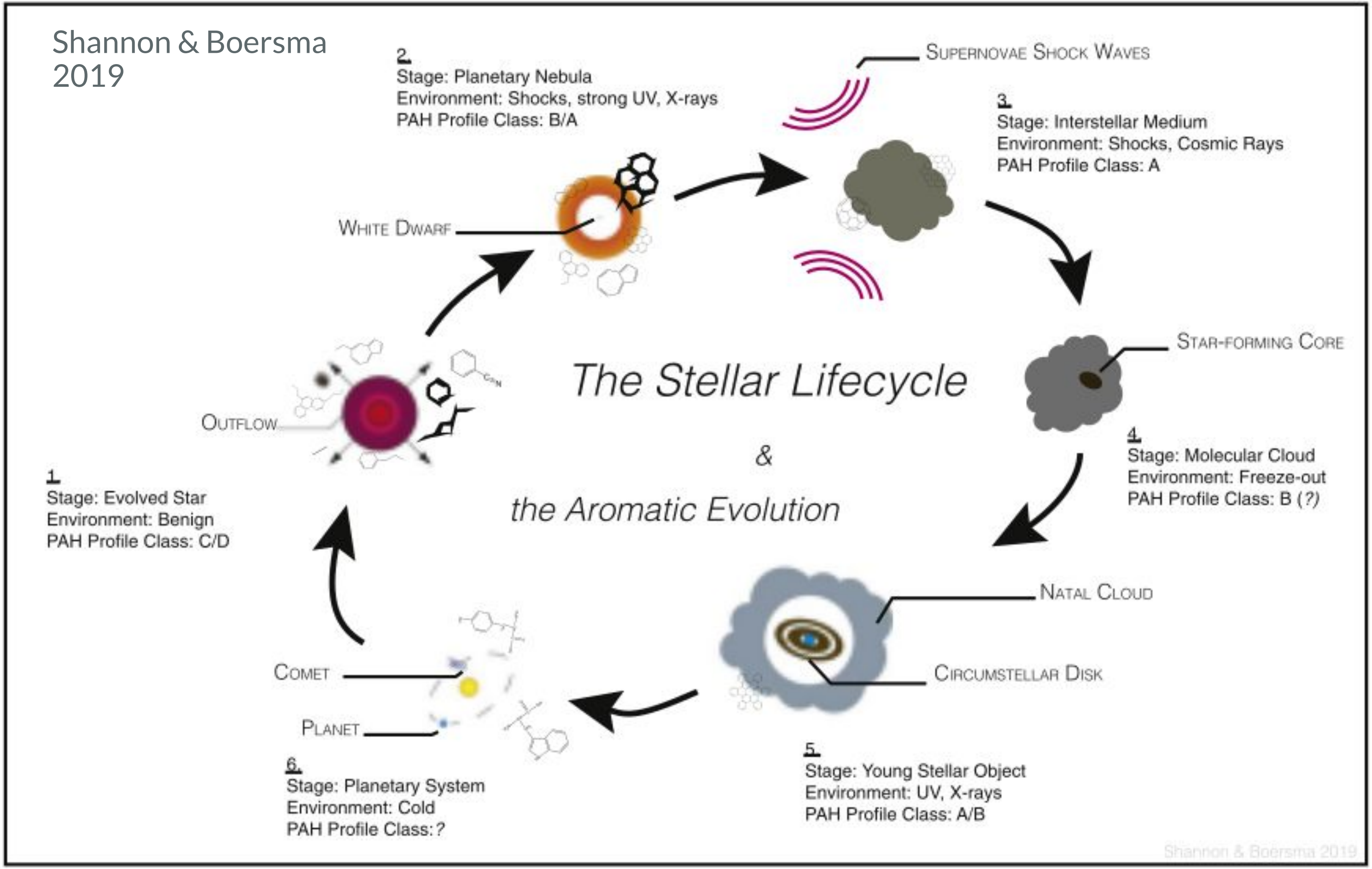


Different kinds of PAH structures (Andrews et al., 2015)

Proposed evolution of PAHs and carbonaceous molecules
(Andrews et al., 2015)

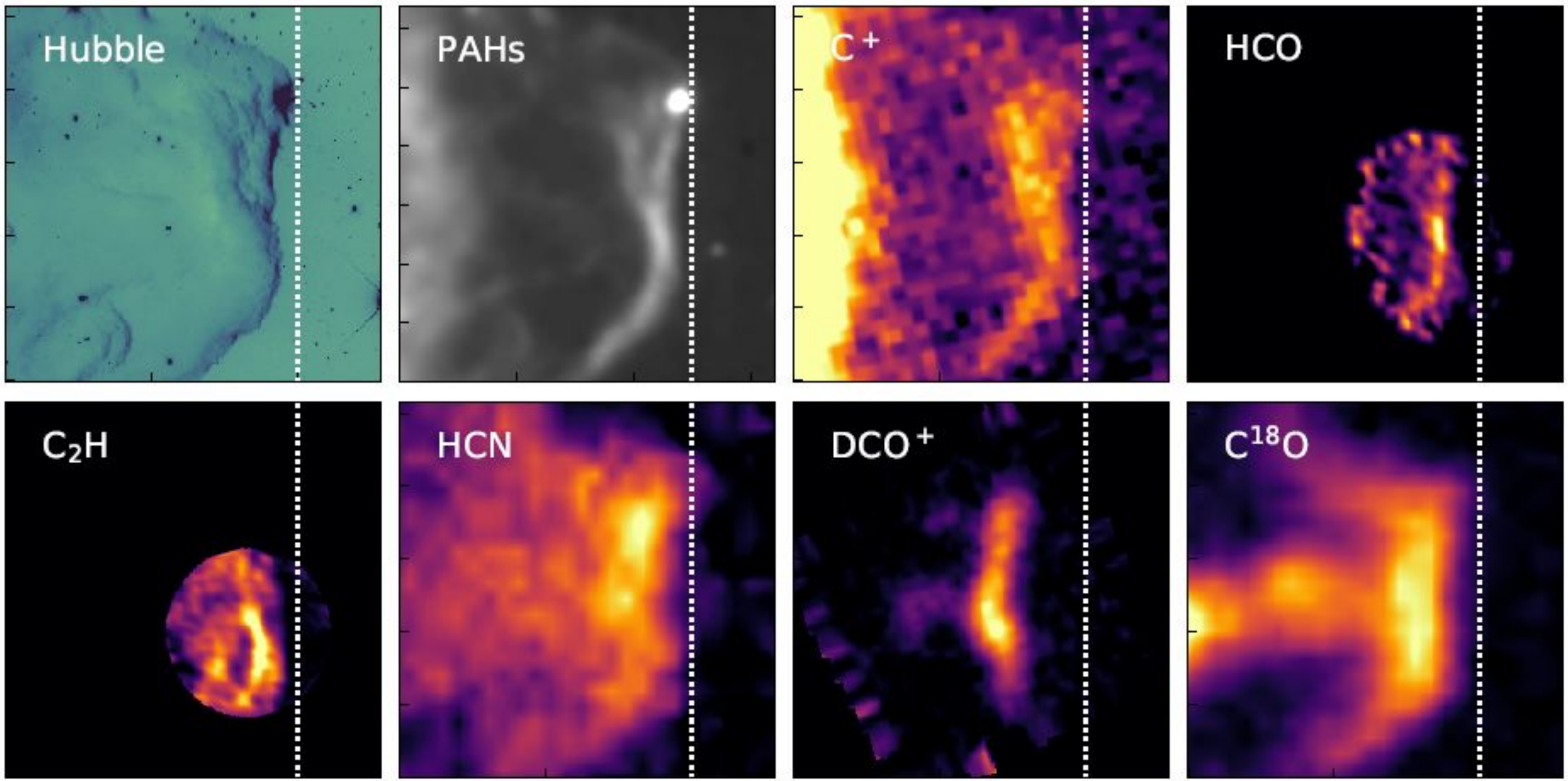


Shannon & Boersma 2019



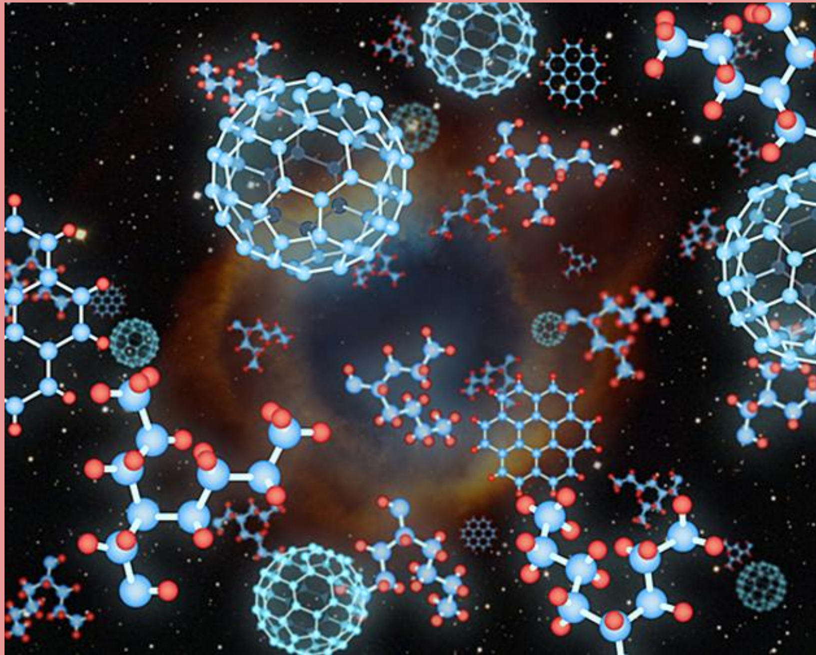
Molecular clouds - Star nurseries

Horsehead Nebula



(Öberg & Bergin 2020, and references therein)

Aromatic molecules in the MIR



6.2, 7.7 and 8.6 μm PAH bands

- **PAH profile variations - Peeters' classes**
  (Peeters et al. 2002, 2005)

- **F7.6/F7.8 > 1 → class A**

- ***Class A 6.2 μm → PANHs**
  (Hudgins et al. 2005)

- **Another reservoir of N**
  (e.g. Canelo 2016)

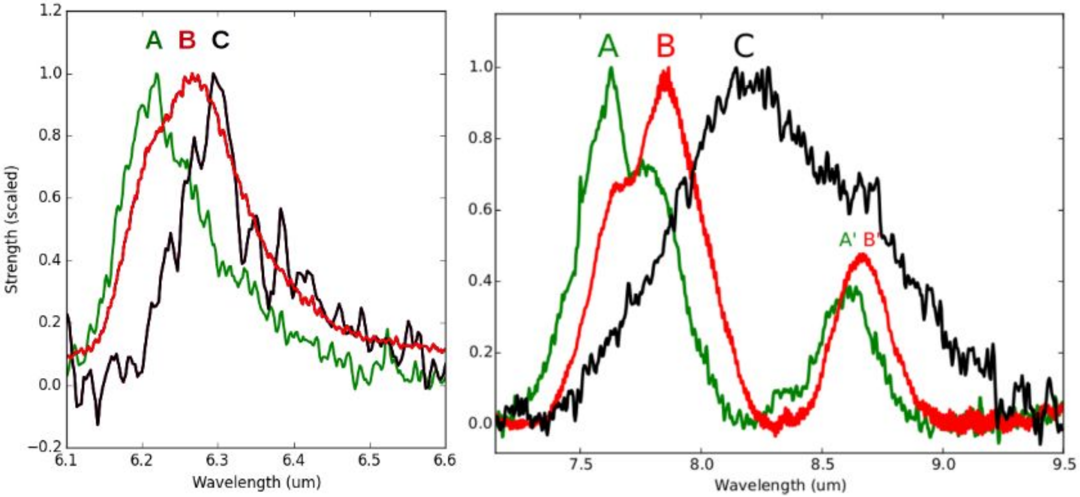


Fig.: Overview of possible variations in the profile of the PAH bands 6.2, 7.7 and 8.6 μm, divided into three classes - A, B and C (Peeters et al., 2002; van Diedenhoven et al., 2004).

Monthly Notices
of the
ROYAL ASTRONOMICAL SOCIETY

MNRAS **475**, 3746–3763 (2018)
Advance Access publication 2018 January 4

doi:10.1093/mnras/stx3351

Variations in the 6.2 μm emission profile in starburst-dominated galaxies: a signature of polycyclic aromatic nitrogen heterocycles (PANHs)?

Carla M. Canelo,[1★] Amâncio C. S. Friaça,[1] Dinalva A. Sales,[2] Miriani G. Pastoriza[3] and Daniel Ruschel-Dutra[4]

[1] *Departamento de Astronomia, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, 05508-090 São Paulo, Brazil*
[2] *Instituto de Matemática, Estatística e Física, Universidade Federal do Rio Grande, 96201-900 Rio Grande do Sul, Brazil*
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Rio Grande do Sul, Brazil*
[4] *Centro de Física e Matemática, Universidade Federal de Santa Catarina, 88040-900 Santa Catarina, Brazil*

Starburst galaxies

Fig.: Starburst galaxy of NGC 3256.

Star formation rate

Milky Way → ~ 3 $M_\odot$/year

Starburst → > 100 $M_\odot$/year

↓

High luminosity in IR

Strong PAH emission

Starburst-dominated galaxies

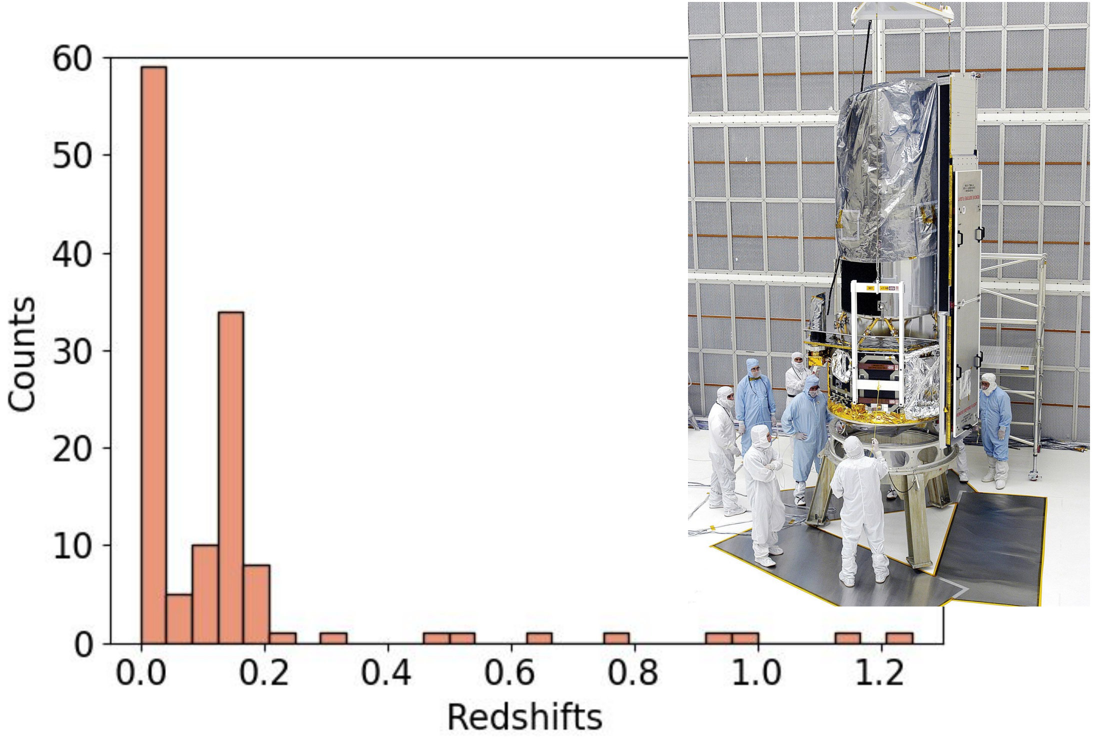


Fig.: Histogram of the redshifts of the 126 selected galaxies (Canelo et al. subm).

126 selected sources

Spitzer/IRS ATLAS project
(Hernán-Caballero & Hatziminaoglou, 2011)

Different types

- **Starburst**
- **ULIRG**
- **Seyfert**
- **LINER**
- ...

Local spline

continuum subtraction

(Canelo et al. subm)

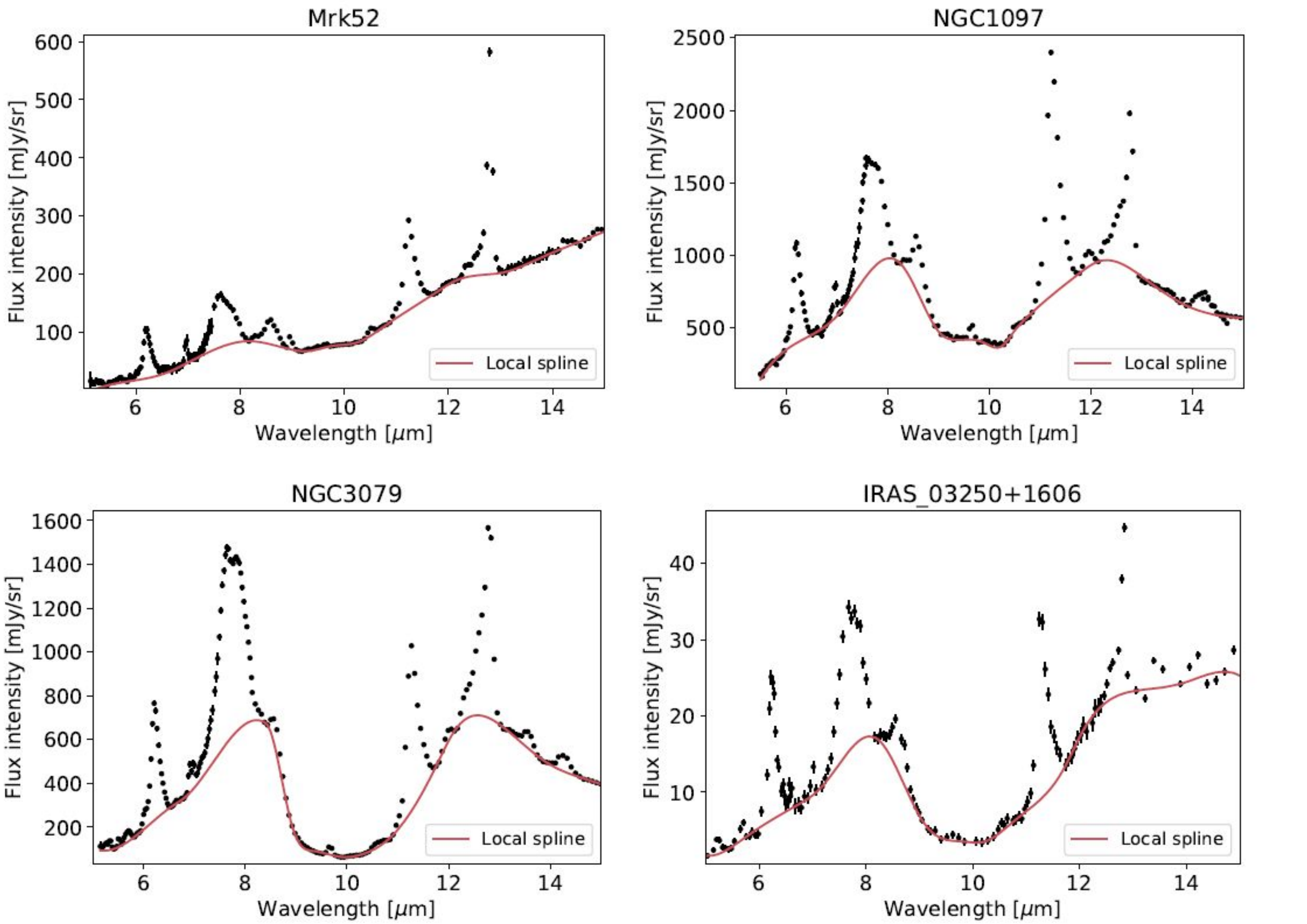


Figure 2. Local spline decomposition of the continuum emission represented by the red line for four objects. The data points are represented by the dots with the vertical error-bars as uncertainties.

Data Analysis - 6 - 9 μm PAH bands

- Python based script → tool curve_fit

- Gaussian profiles:
  - 6.2 μm
  - 7.6 and 7.8 μm

  *fixed FWHM

  - 8.6 μm

independent fitting

Tab.: Intervals for each Peeters' classes (Peeters et al. 2002).

Class	6.2 μm	7.7 μm	8.6 μm
A	< 6.23	~ 7.6 $(F_{7.6}/F_{7.8} \geq 1)$	< 8.6
B	$6.23 < \lambda < 6.29$	~ 7.8 $(F_{7.6}/F_{7.8} < 1)$	> 8.6
C	> 6.29	~ 8.22	——

$$I_{gauss} = \frac{A}{\sigma\sqrt{2\pi}} exp\left(-\frac{(x-\lambda_c)^2}{2\sigma^2}\right)$$

6.2 µm PAH band

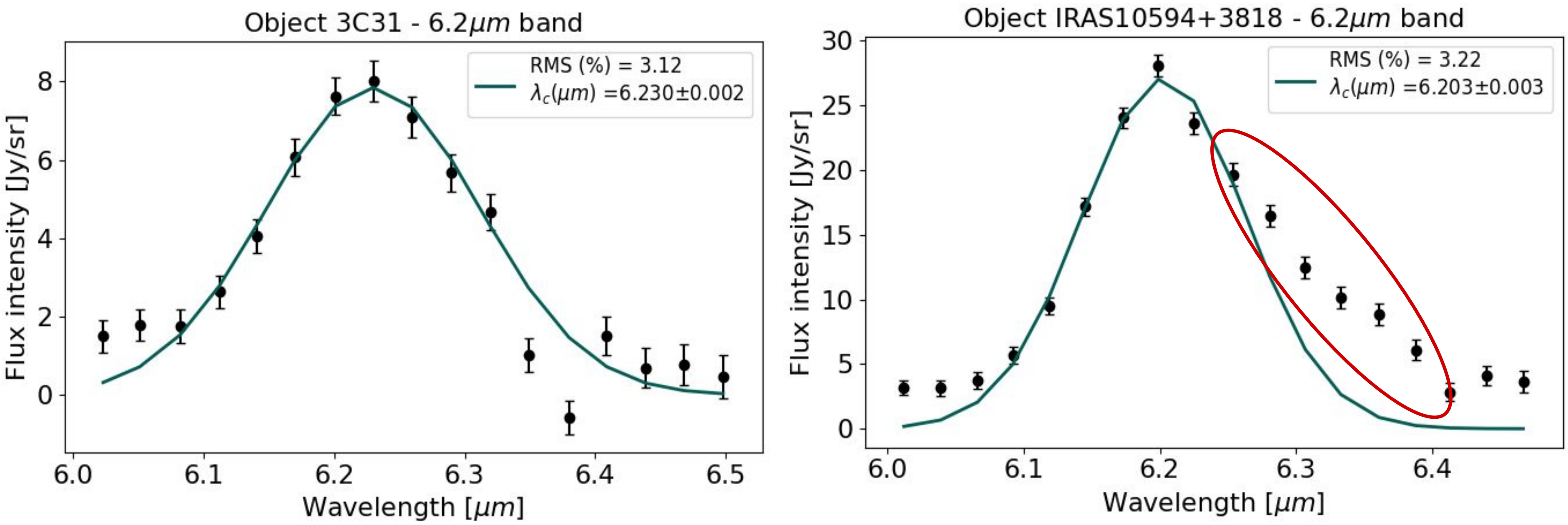
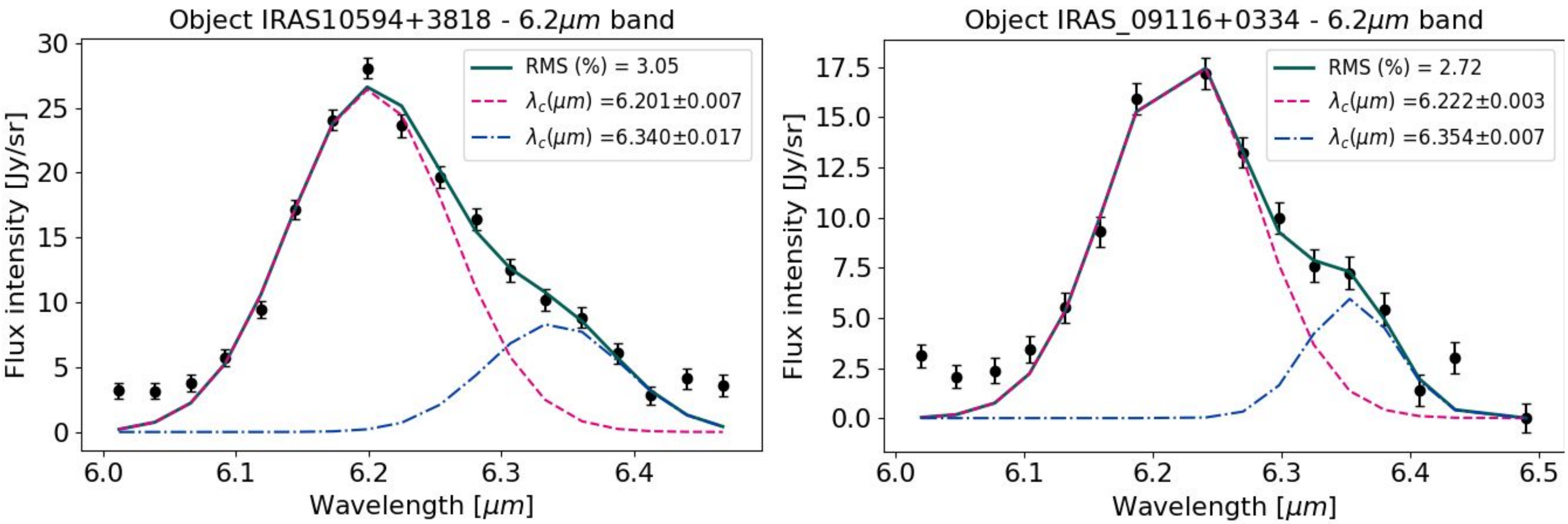


Fig.: Profiles of 6.2µm band for two sources (Canelo et al. 2018).

- Red tail → asymmetric profile (e.g. Tielens et al. 2008)

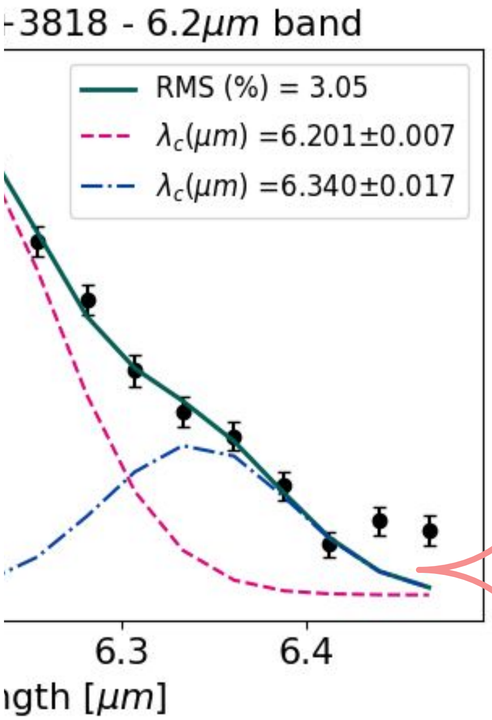
6.2 μm PAH band



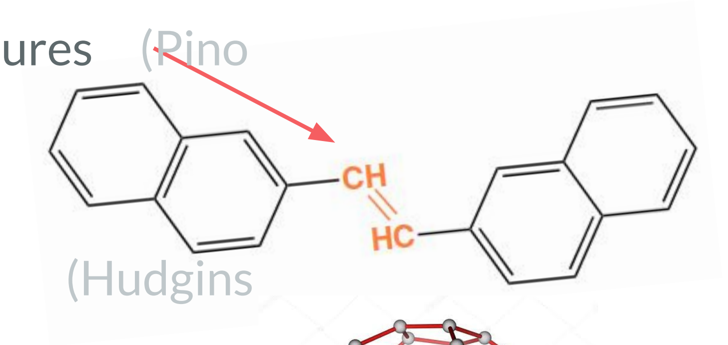
- Or another feature?

Fig.: Profiles of the 6.2μm band for two sources using two Gaussians (Canelo et al. 2018).

6.2 μm PAH band

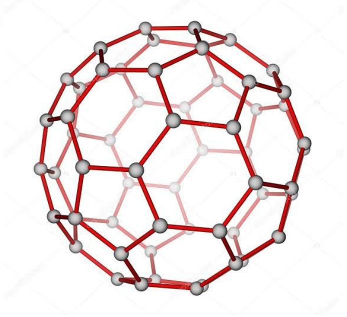


- 6.3 μm → aliphatic features (Pino et al. 2008)

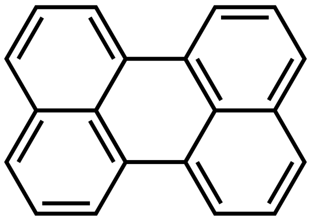


- PAH cations (Hudgins et al. 2005)

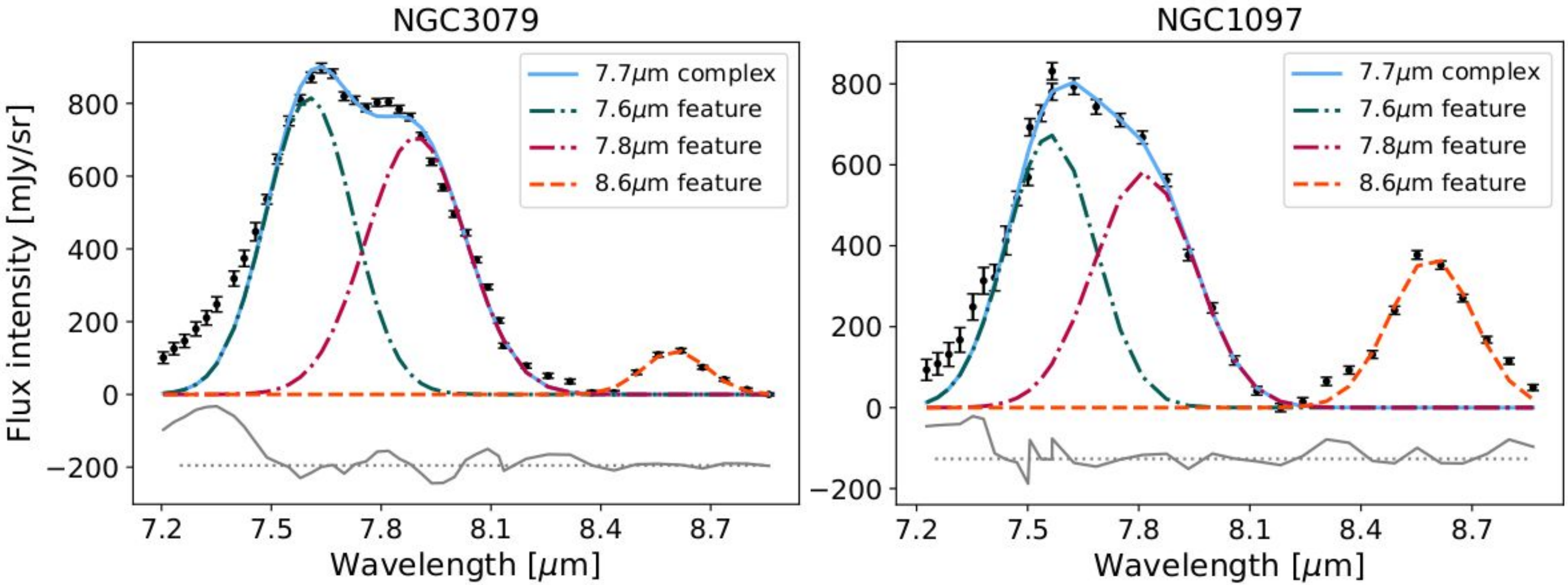
- 6.4 μm → $C^{+}60$ (Berné, Montillaud & Joblin 2015)



- Perylene-like structures (Candian, Sarre & Tielens 2014)



7.7 and 8.6 μm PAH band (Canelo et al. subm.)



- Fainter PAH features at 7.4 and 8.33 μm (e.g. Smith et al. 2007)

Distribution of the classes - 6.2, 7.7 e 8.6 μm

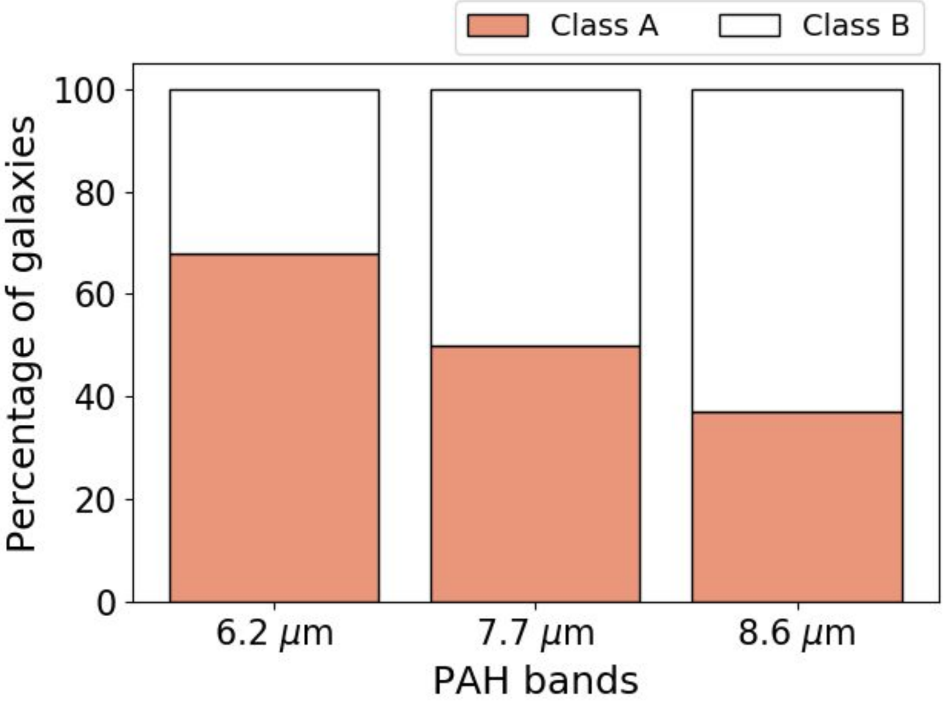


Fig.: Histogram of the classes' distribution (Canelo et al. subm.).

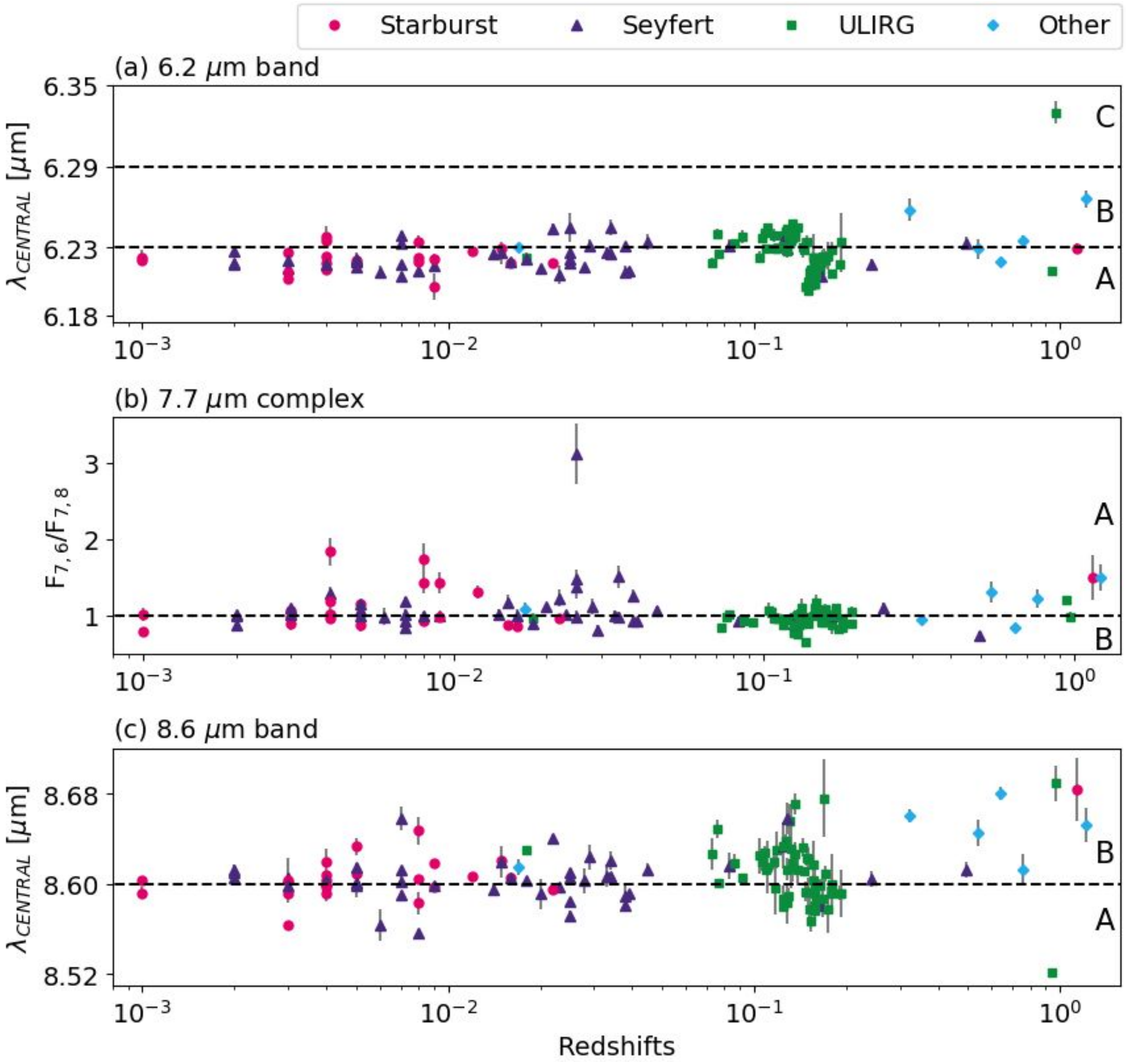
Tab.: Classes' distribution (Canelo et al. submitted).

Band (μm)	Class A (per cent)	Class B (per cent)	Class C (per cent)
6.2	68	31	1
7.7	50	50	—
8.6	37	63	—

6.2 μm → "A" – 68%

- PANHS

(Canelo et al. 2018, subm.)



- more class B sources in higher redshifts

- possible PAH evolutionary timescale

(e.g. aromatic evolution in stellar lifecycle, Shannon & Boersma, 2019)

Fig.: Distribution of the PAH bands into Peeters' classes according to the galaxies redshift (Canelo et al. subm.).

The hot molecular core G331.512-0.103

Hot molecular core (G331)

- ~7.5 kpc
- outflow with 55 M☉
- n(H2) ≈ 10^7 cm^{-3}
- v_{lsr} ~ -90 km/s

- Shell-like structure
  - CH3CN → Tkin ~ 141 K
  - HC3N → Tkin ~ 90 K
  - CH3OH → Tkin ~ 74 K

(Mendoza et al. 2018, Duronea et al. 2019, Hervías-Caimapo et al. 2019)

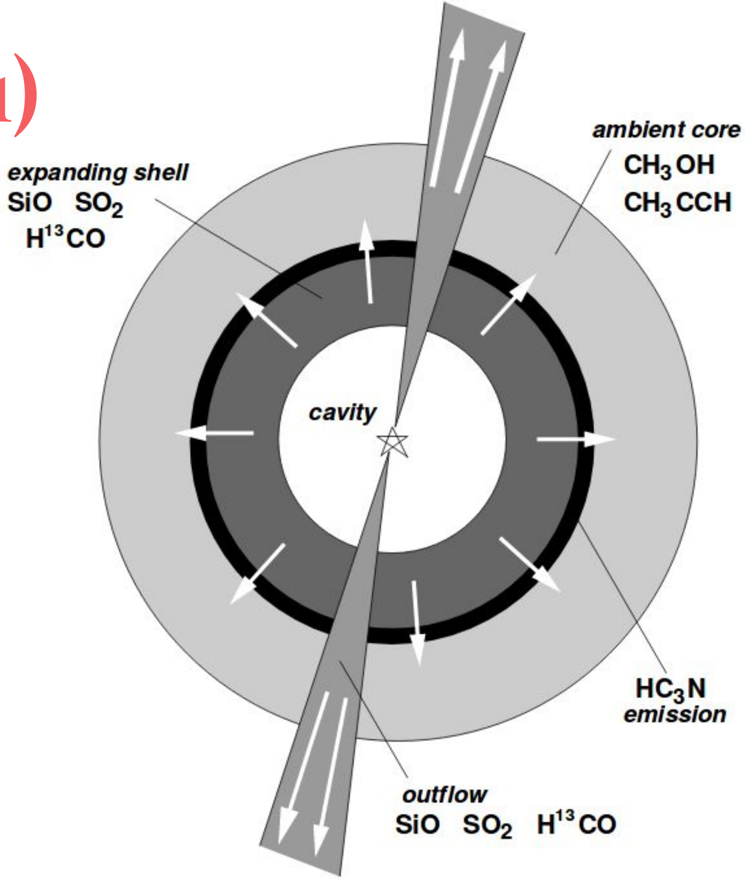


Figure 8. Sketch of the simple model proposed to explain the emission of HC_3N and other molecules detected in G331 (based on the models of Merello et al. 2013a and Hervías-Caimapo et al. 2019).

Data Analysis

- CLASS/GILDAS software*
- Line identification
    - Ta < 1 K
- Databases: CDMS, JPL, Splatalogue and NIST

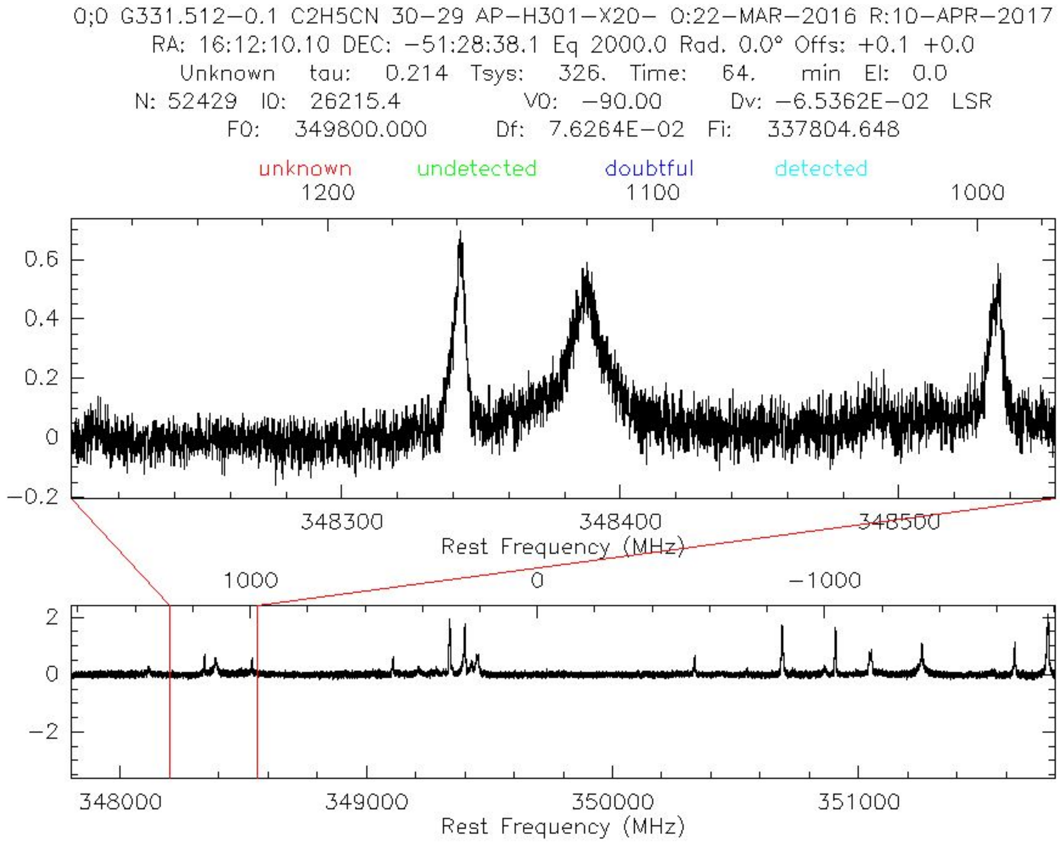


Fig.: Observed spectral bands of G331 with a frequency of 347.8 to 351.8 GHz.

*https://www.iram.fr/IRAMFR/GILDAS/

Preliminar line identification

- Several possible COMs: CH3OCH3, CH3OCHO, C2H5CN and C3H7CN
- HNCO
- formamide may have not been detected

Tabela 4.2 - Análise espectral preliminar das linhas de emissão observadas em G331 com APEX-2. Espécies com asterisco indicam que as respectivas transições estão presentes no NIST.

Espécie	Transição	Frequência (MHz)	$A_{i,j}$ (s^{-1})	E_{up} (K)	T_a (K)	Contaminantes
CH3OCH3*	16 116 3–15 015 3 16 116 5–15 015 5 16 116 1–15 015 1 16 116 0–15 015 0	292412.244 292412.416 292412.588	1.97E-04	120.3	0.787	CH3C-13-H2CN. Glycine
SO-17	7 8 6–6 7 6 7 8 7–6 7 7	292432.984 292438.495	1.75e-05 2.37e-05	59.9	0.607	CH2CHCNH+
CH3CH(NH2)CN	22 913–21 714 22 617–21 418	292464.630 292466.840	1.16e-05 7.42e-06	104.4 94.3	0.613	trans-propenal. ag-diethyl ether
CH3OH	6 1 5 -0–5 1 4 -0	292672.89	1.06E-04	63.7	2.133	Oxetane. aa-diethyl ether. Propynal. Benzyne
H2CN	4 0 4 8 5–3 0 3 8 4 4 0 4 2 6–3 0 3 2 5	292825.591 292828.963	7.79e-04 8.12e-04	35.2	0.72	CH3C-13-H2C-13-N. ag-diethylether. HOCH2CN
SO2	13 6 8–14 5 9	292882.697	3.74E-05	171.9	0.749	Propene
H2C-13-O*	4 1 3–3 1 2	293126.515	6.64E-04	47	1.391	CH3C-13-H2C-13-N. Benzyne
CH3OH*	3 2 1 +0–4 1 4 +0	293464.203	2.86E-05	51.6	0.991	S-33-O. HC(O)NH2. CH2(OH)CDO
S-34-O2	19 317–19 218	293481.705	1.90E-04	195.9	0.747	H2CND. CH2(OD)CHO. H2CNCH2CN

Continua na próxima página. . .

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS **504,** 4428–4444 (2021) doi:10.1093/mnras/stab1163
Advance Access publication 2021 April 23

Isocyanic acid (HNCO) in the hot molecular core G331.512-0.103: observations and chemical modelling

Carla M. Canelo,[1★] Leonardo Bronfman,[2★] Edgar Mendoza,[1,3★] Nicolas Duronea,[4] Manuel Merello,[2] Miguel Carvajal,[5,6] Amâncio C. S. Friaça[1] and Jacques Lepine[1]

[1]*Departamento de Astronomia, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, São Paulo, 05508-090, Brazil*
[2]*Departamento de Astronomía, Universidad de Chile, Casilla 36-D, Santiago de Chile, Chile*
[3]*Observatório do Valongo, Universidade Federal do Rio de Janeiro, Ladeira Pedro Antônio, 43, Rio de Janeiro, RJ 20.080-090, Brazil*
[4]*Instituto de Astrofísica de La Plata (UNLP - CONICET), La Plata, Argentina*
[5]*Dept. Ciencias Integradas, Facultad de Ciencias Experimentales, Centro de Estudios Avanzados en Física, Matemática y Computación, Unidad Asociada GIFMAN, CSIC-UHU, Universidad de Huelva, Spain*
[6]*Instituto Universitario Carlos I de Física Teórica y Computacional, Universidad de Granada, Spain*

Accepted 2021 April 20. Received 2021 April 20; in original form 2021 January 27

HNCO K=0

- CH3OH (OMC-1, Loren & Mundy 1984)

- *SO2, OC(CN)2, HCCCH2NH2, or H2CNCH2CN

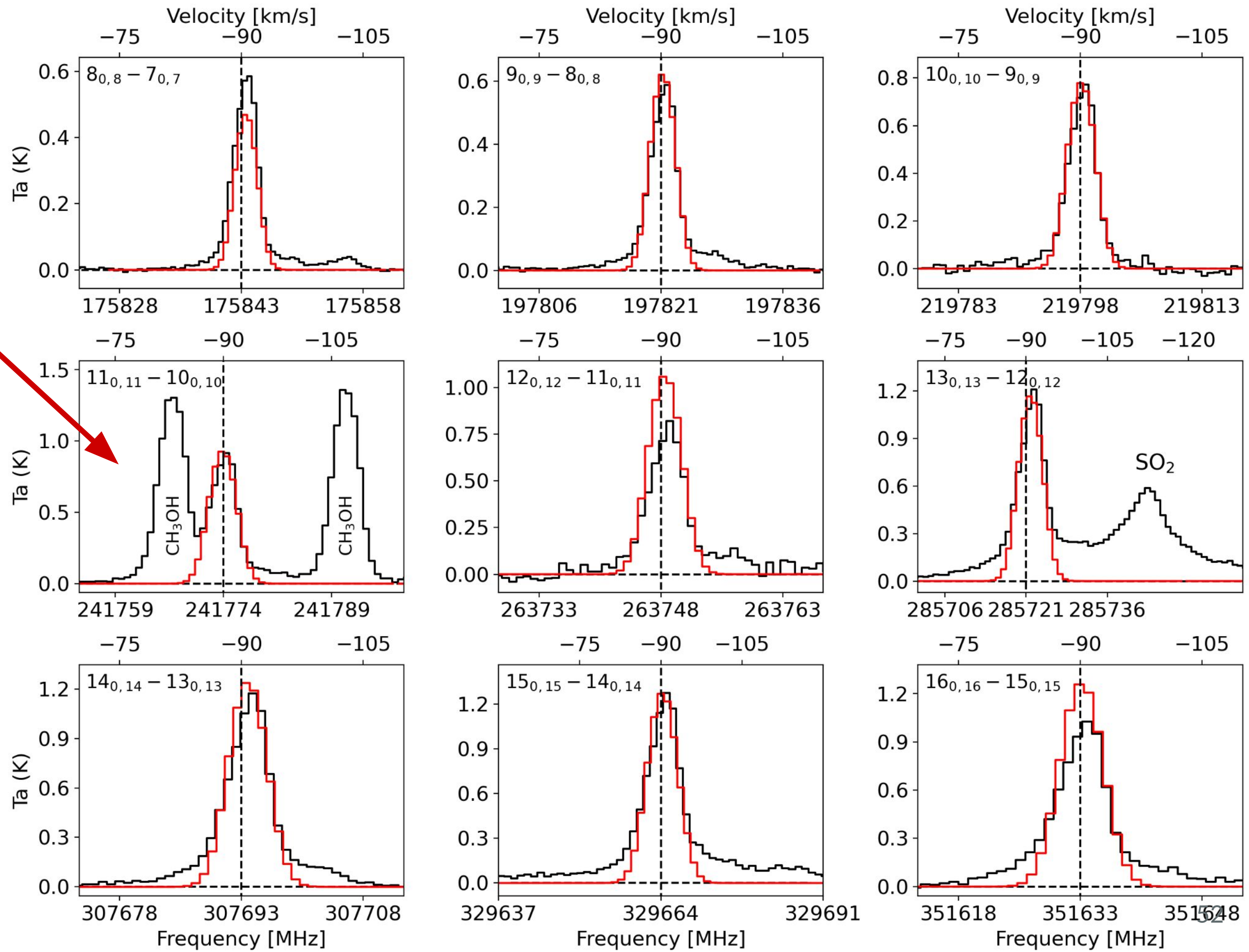


Fig.: HNCO emission lines (K=0) with a resolution of 1 km/s (Canelo et al. 2021).

Rotational diagram

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N}{Z}\right) - \frac{E_u}{kT_{exc}}$$

(Goldsmith & Langer 1999)

Texc = 59.4 ± 2.3 K

N = 3.1 ± 0.4 x 10^{15} cm^{-2}

*Opacity correction

Texc = 58.8 ± 2.7 K

N = 3.7 ± 0.5 x 10^{15} cm^{-2}

- T ~ 60 K → HNCO in external regions of G331

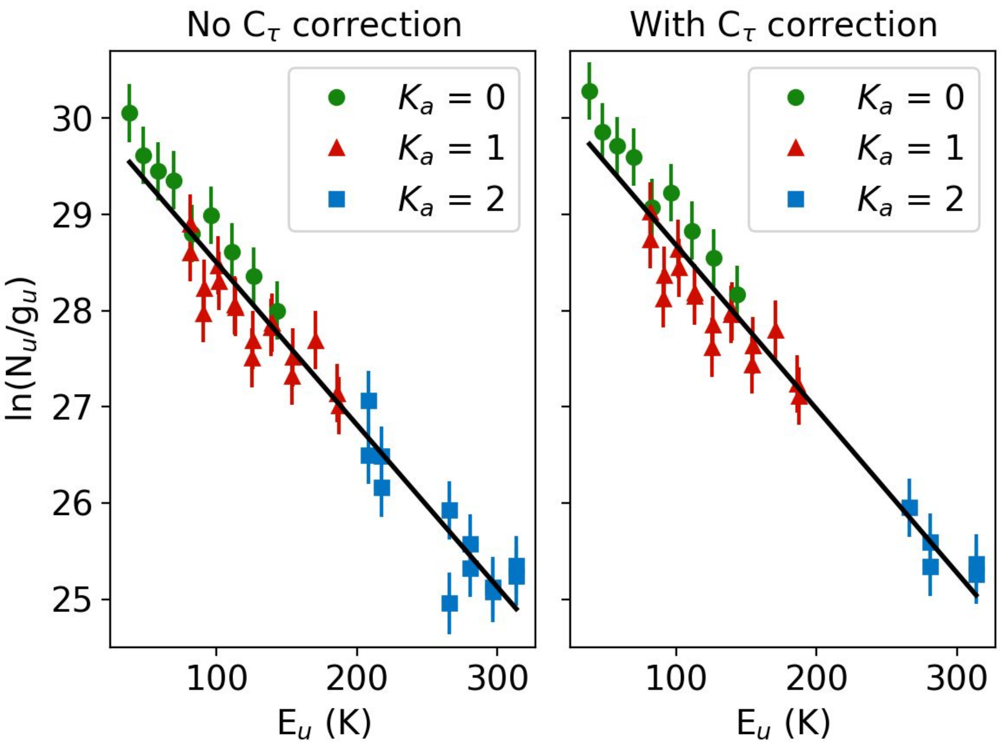


Fig.: Rotational diagram of HNCO to a source size of 5 arcsec (Canelo et al. 2021).

NAUTILUS chemical simulation

- T = 60 K reproduces the observed abundances

- Chemical age ~10^5 yr

- Dynamical age ~ 10^3 yr (Merello et al. 2013)

❖ 0D- simulations
❖ formation reactions (NH + CO → HNCO)

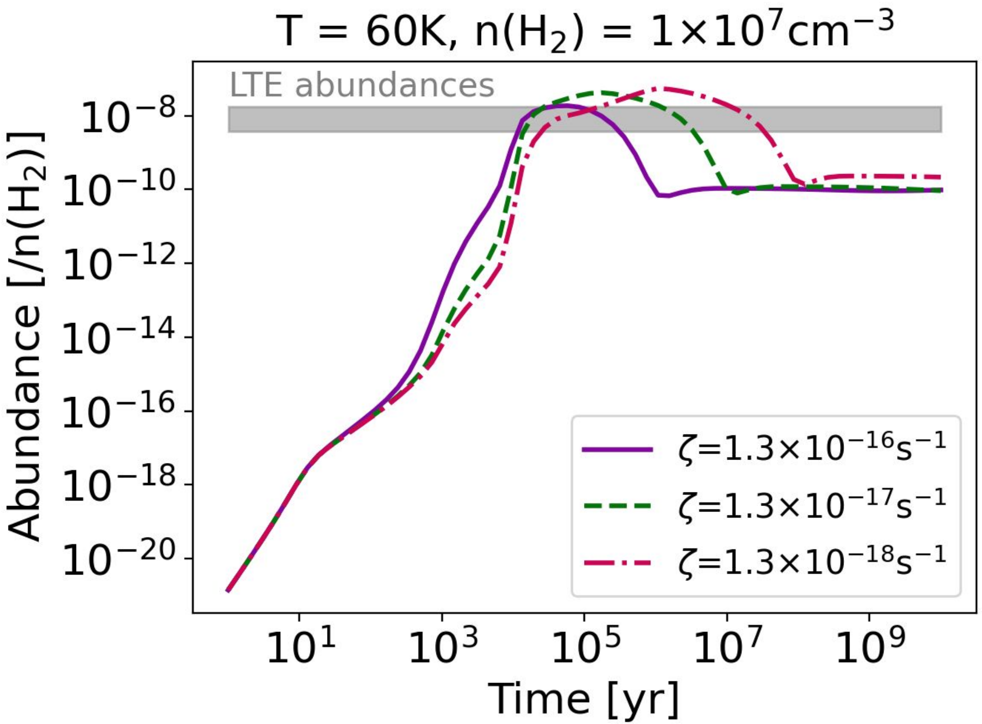


Fig.: Best-fit time evolution of the HNCO abundances simulated with NAUTILUS (Canelo et al. 2021).

Final remarks

Final remarks

- Chemical probes are essential to understand the formation of the first stars in the early universe, the origin of today's stars and planets, and the emergence of life on Earth and elsewhere.

- A multi-field approach is important to better understand the chemical complexity in the Universe

- PANHs could dominate the 6.2μm band emission
- Possible PAH evolution in galaxies along to redshifts

- G331 presents a high chemical complexity
- 42 lines of HNCO were detected in G331 with T ~ 60K

Thank you!

camcanelo@gmail.com