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A: Glad you could join us!
Q: Good afternoon! I'm joining from Murfreesboro, TN.
A: Good to see you here.
Q: Hello! Doug here, Redding California.
A: Good to see you here Doug!
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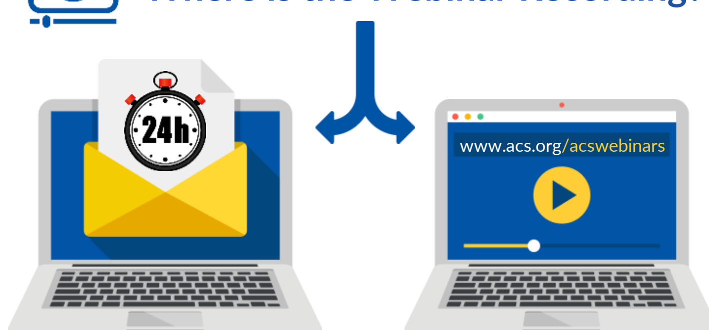

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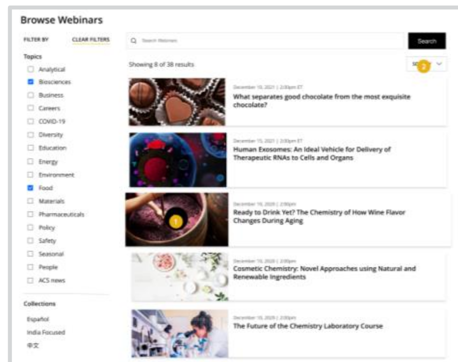

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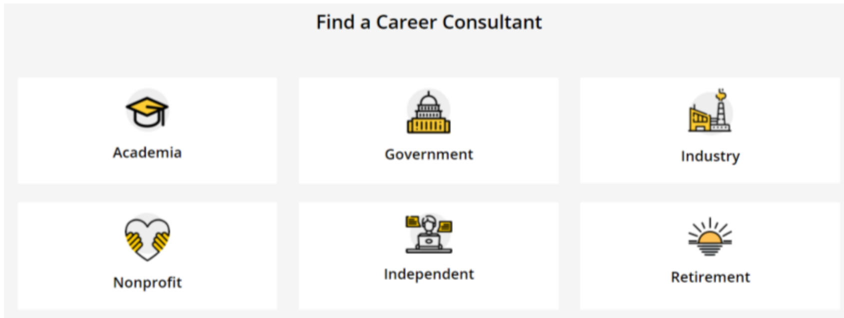

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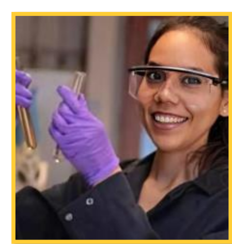

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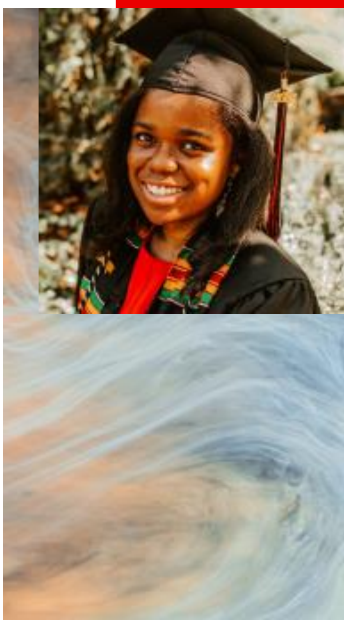

ACS Scholar Adunoluwa Obisesan

BS, Massachusetts Institute of Technology, June 2021
(Chemical-biological Engineering, Computer Science & Molecular Biology)

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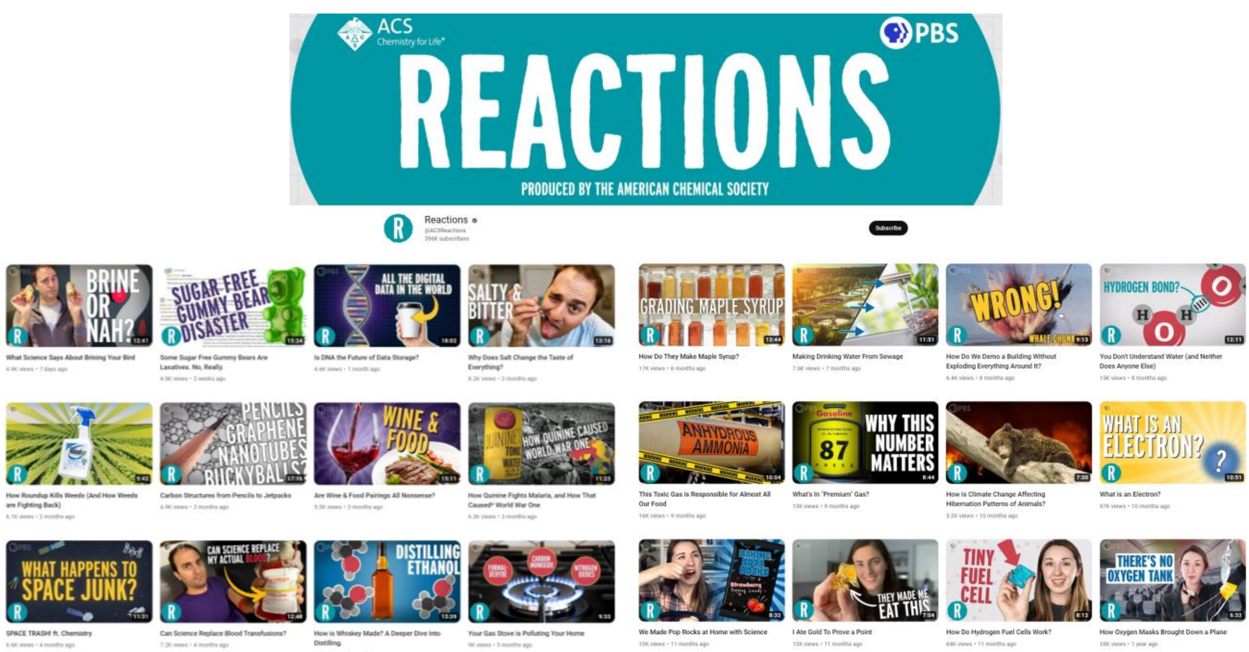

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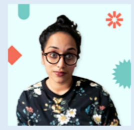
Sam Jones, PhD
Science Writer & Exec Producer



Deboki Chakravarti, PhD
Science Writer & Co-Host

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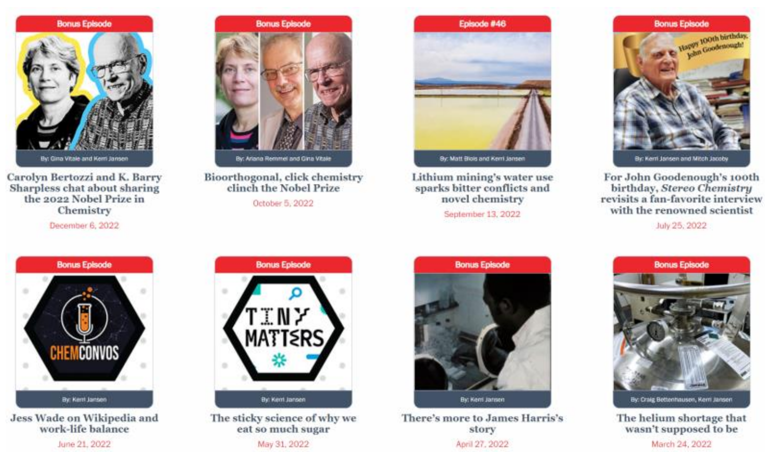

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ACS ON CAMPUS

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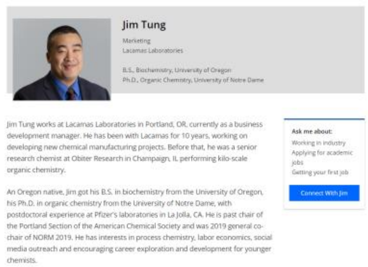

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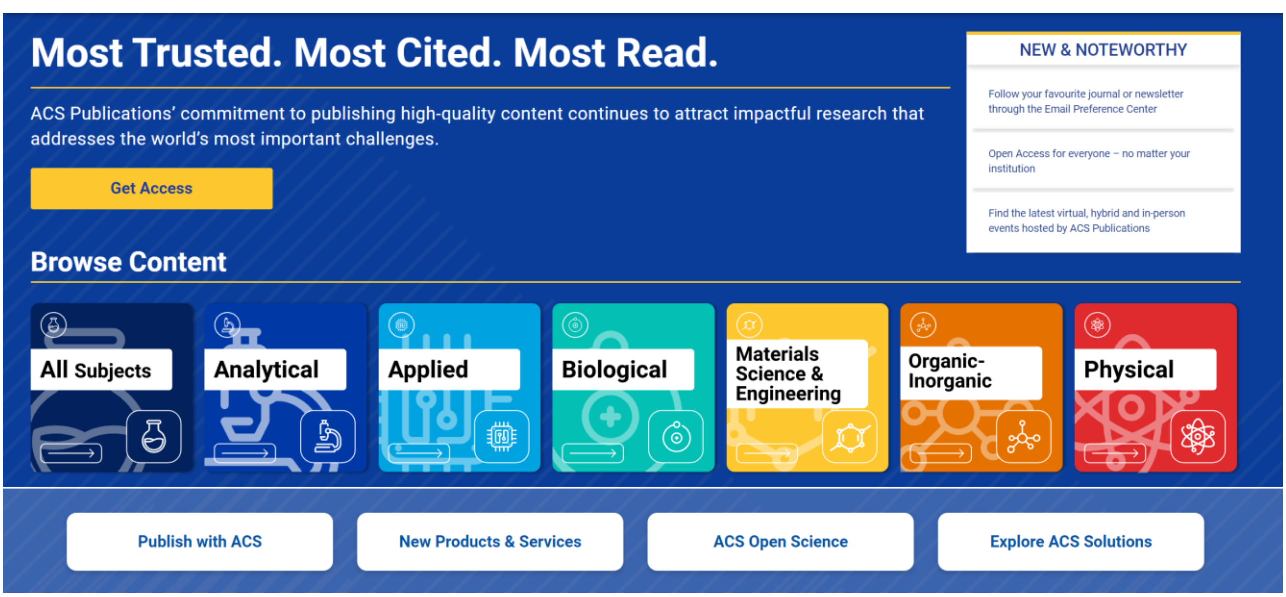

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The impact and results of **ACS member advocacy** outreach and efforts by the numbers!

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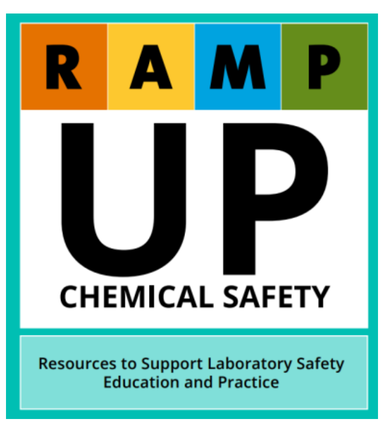
ACS Committee Chemical Safety

A complete listing of ACS Safety Programs and Resources



Download it for free in the "Projects & Announcements" Section! www.acs.org/ccs

ACS OFFICE OF DEIR

Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect

Resources

Inclusivity Style Guide
Designed to help staff and members use language and images that respect diversity in all its forms.

ACS Webinars on Diversity
Covering diversity and inclusion at the workplace

ACS Publications DEIR Hub
See what ACS Publications is doing for fostering inclusivity in scholarly publishing

ACS Volunteer and ACS Meetings Code of Conduct
Fostering a positive and welcoming environment for attendees, volunteers and staff.

C&EN Trailblazers
C&EN highlights scientists from different backgrounds who are making an impact in chemistry.

NEW! Download DEIR Educational Resources
Download this educational guide for additional recommendations on videos, articles, books, podcasts, and more on diversity, inclusion, and related topics.

Quick Guide: Inclusion Moments
Learn more about what Inclusion Moments are and see ideas to host them during your meetings.

Quick Guide: How to host inclusive in-person events
Recommendations and best practices to ensure that your events can accommodate everyone.

Diversity, Equity, Inclusion, and Respect

**Adapted from definitions from the Ford Foundation Center for Social Justice:

Equity**
Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe this is only possible in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented the full participation of some groups.

Diversity**
The representation of varied identities and differences (race, ethnicity, gender, disability, sexual orientation, gender identity, national origin, tribe, caste, socio-economic status, thinking and communication styles, etc.), collectively and as individuals. ACS seeks to proactively engage, understand, and draw on a variety of perspectives.

Inclusion**
Builds a culture of belonging by actively inviting the contribution and participation of all people. Every person's voice adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be called upon to represent an entire community.

Respect
Ensures that each person is treated with professionalism, integrity, and ethics underpinning all interpersonal interactions.

https://www.acs.org/diversity

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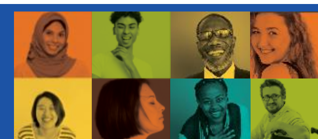

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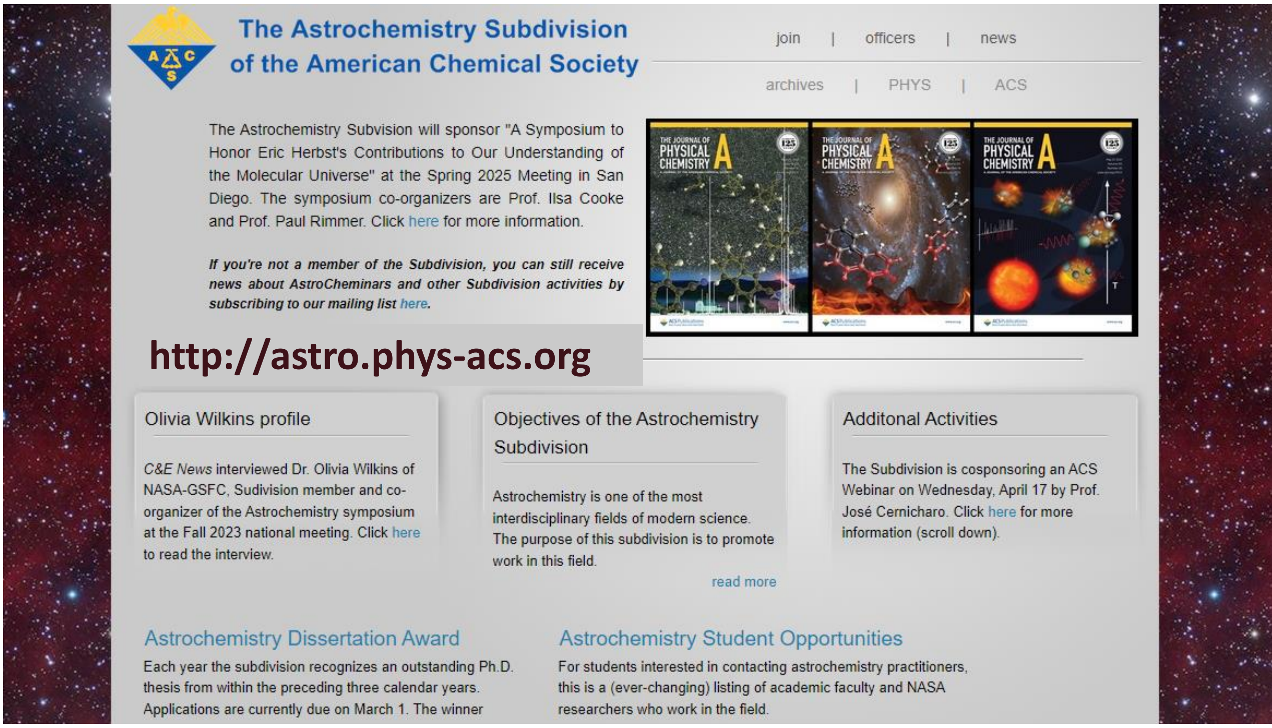

The Astrochemistry Subdivision
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The Astrochemistry Subvision will sponsor "A Symposium to Honor Eric Herbst's Contributions to Our Understanding of the Molecular Universe" at the Spring 2025 Meeting in San Diego. The symposium co-organizers are Prof. Ilsa Cooke and Prof. Paul Rimmer. Click here for more information.
If you're not a member of the Subdivision, you can still receive news about AstroCheminars and other Subdivision activities by subscribing to our mailing list here.
http://astro.phys-acs.org
THE JOURNAL OF PHYSICAL CHEMISTRY A
Olivia Wilkins profile
C&E News interviewed Dr. Olivia Wilkins of NASA-GSFC, Sudivision member and co-organizer of the Astrochemistry symposium at the Fall 2023 national meeting. Click here to read the interview.
Objectives of the Astrochemistry Subdivision
Astrochemistry is one of the most interdisciplinary fields of modern science. The purpose of this subdivision is to promote work in this field.
read more
Additonal Activities
The Subdivision is cosponsoring an ACS Webinar on Wednesday, April 17 by Prof. José Cernicharo. Click here for more information (scroll down).
Astrochemistry Dissertation Award
Each year the subdivision recognizes an outstanding Ph.D. thesis from within the preceding three calendar years. Applications are currently due on March 1. The winner
Astrochemistry Student Opportunities
For students interested in contacting astrochemistry practitioners, this is a (ever-changing) listing of academic faculty and NASA researchers who work in the field.

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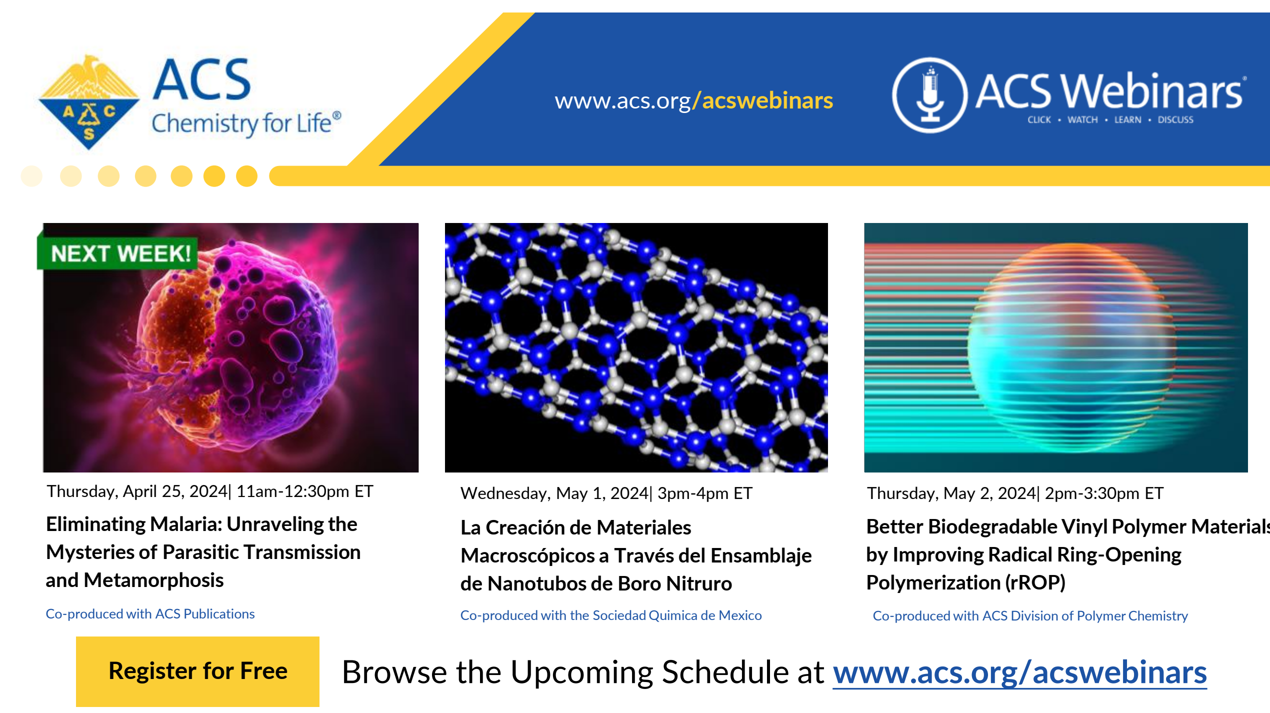

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Thursday, April 25, 2024| 11am-12:30pm ET
Eliminating Malaria: Unraveling the Mysteries of Parasitic Transmission and Metamorphosis
Co-produced with ACS Publications
Wednesday, May 1, 2024| 3pm-4pm ET
La Creación de Materiales Macroscópicos a Través del Ensamblaje de Nanotubos de Boro Nitruro
Co-produced with the Sociedad Quimica de Mexico
Thursday, May 2, 2024| 2pm-3:30pm ET
Better Biodegradable Vinyl Polymer Materials by Improving Radical Ring-Opening Polymerization (rROP)
Co-produced with ACS Division of Polymer Chemistry
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THIS ACS WEBINAR® WILL BEGIN SHORTLY…

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Astrochemistry's New Golden Age: Finding New Molecules In Space With Ultrasensitive Molecular Line Surveys

JOSÉ CERNICHARO, PhD

Professor of Investigación,
Instituto de Física Fundamental (CSIC)

ANTHONY REMIJAN, PhD

Assistant Director, Science Support and
Research, National Radio Astronomy Observatory

This ACS Webinar® is co-produced with the ACS PHYS Astrochemistry Subdivision.

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Astrochemistry's New Golden Age:
Finding New Molecules In Space With Ultrasensitive Molecular Line Surveys

J.Cernicharo
Department of Molecular Astrophysics
IFF-CSIC (Madrid, Spain)
jose.cernicharo@csic.es

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- What are the physical conditions of interstellar molecular clouds? Where stars and planets are formed ? How molecules are formed in space?
- Molecular Astrophysics and Astrochemistry
- Molecules as tracers of the physical conditions of molecular clouds
- Line surveys (all wavelengths)
- Molecular spectroscopy in space (QUIJOTE line survey). The NEW golden age of astrochemistry. The formation of PAHs in cold environments (GOTHAM and QUIJOTE)

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List of acronyms and symbols used in the presentation

- ISM: Insterstellar Medium
- CSM: Circumstellar Medium
- n: volume density of H_2 (cm^{-3})
- T_K: Kinetic temperature (K)
- N: column density (cm^{-2})
- NRAO: National Radioastronomy Observatory (USA)
- IRAM: Institute de Radioastronomie millimétrique (France, Germany, Spain)
- Yebes: National Astronomical Observatory (Yebes, Guadalajara; Spain)
- TMC-1: Taurus Molecular Cloud 1 (T_K=10 K, n~10^4 cm^{-3})
- IRC+10216: Carbon-rich reed giant star (CW Leo)
- LTE: Local Thermodynamical equilibrium
- LVG: Large velocity gradient radiative transfer method
- GOTHAM: **GBT Observations of TMC-1: Hunting Aromatic Molecules**
- QUIJOTE: **Q-band Ultrasensitive Inspection Journey to the Obscure TMC-1 Environment**
- CRESU: **Cinétique de Réaction en Ecoulement Supersonique Uniforme** = Reaction kinetics in uniform supersonic flow
- SANCHO: **Surveying the Area of the Neighbour TMC-1 Cloud through Heterodyne Observations** 27
- NANOCOSMOS: **European Research Council Synergy project (funding for QUIJOTE and SANCHO)**

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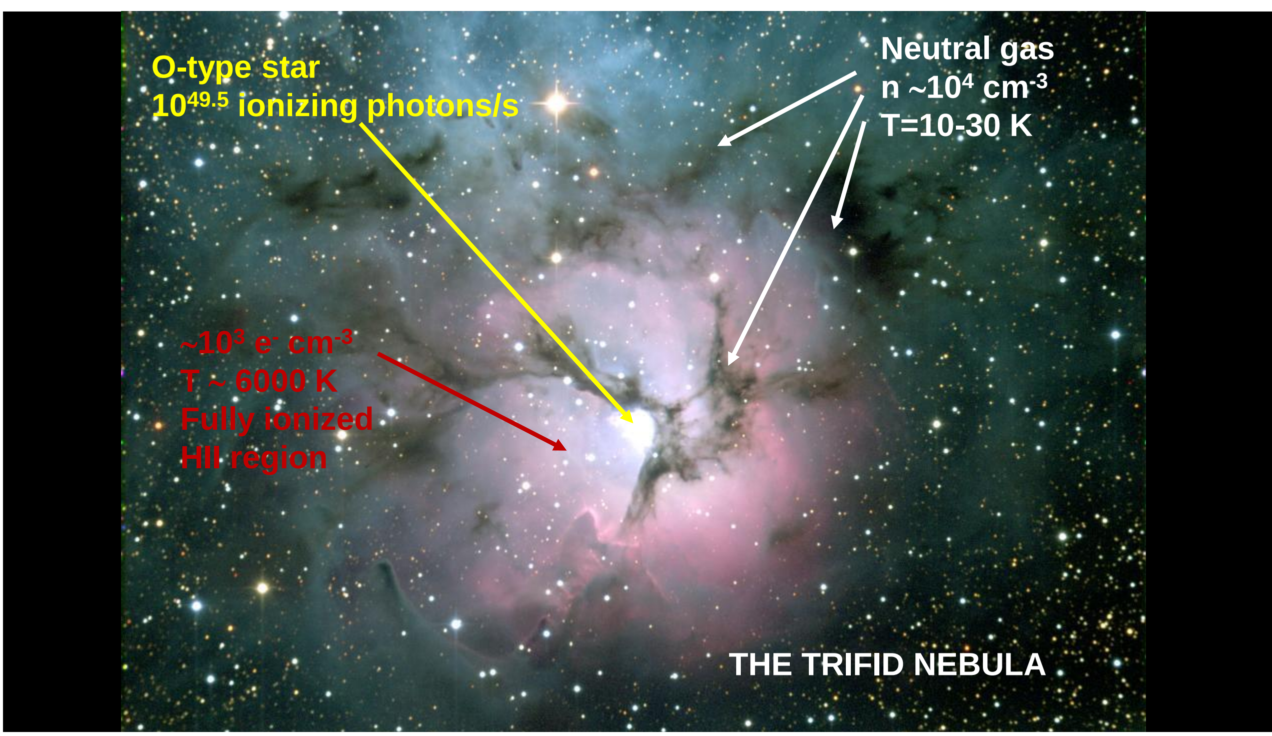

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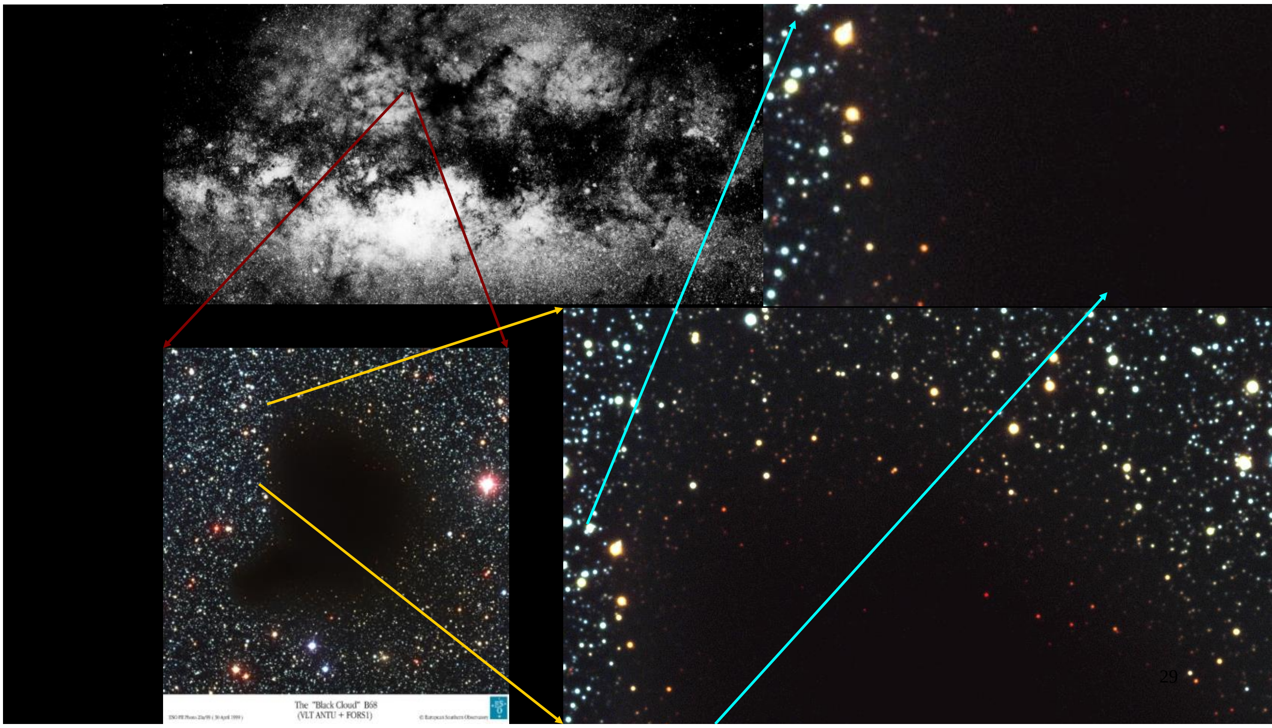

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Clouds are composed of dust and gas.

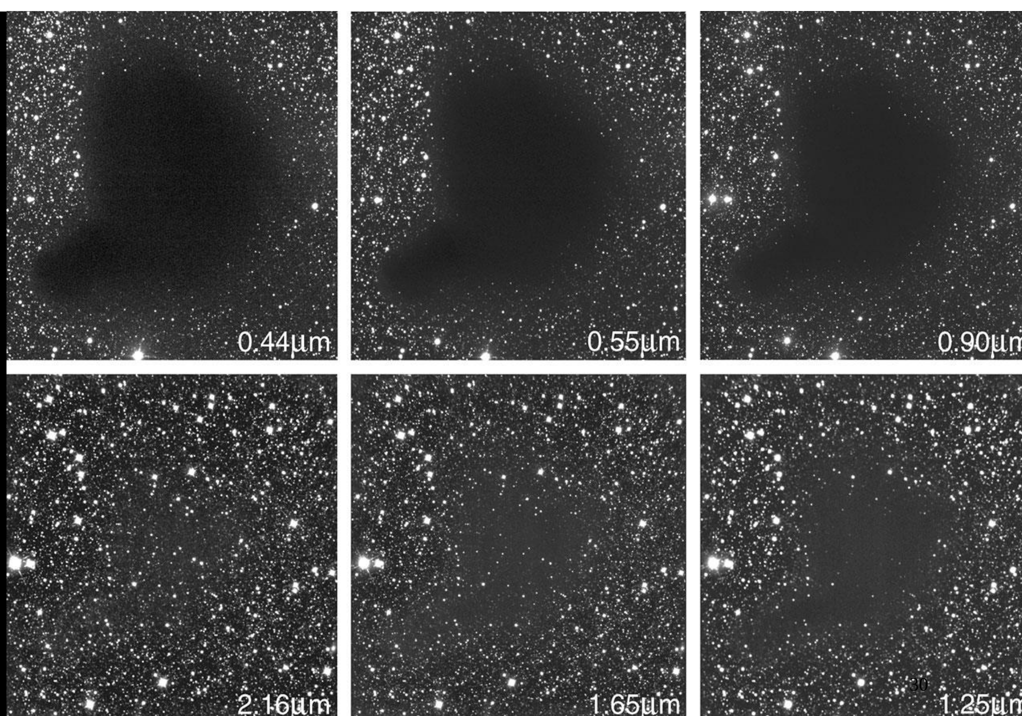
Dust grains have a typical size of 0.5 µm and represent ~1% of the mass

~99% is neutral gas

H_2, CO, HCN, HNC, HCO^+, CN, CH_3CCH, HC_3N,…

H_2 is formed at the surface of dust grains

H_2^+ is produced from H_2 and CR
$H_2 + H_2^+ \Rightarrow H_3^+$



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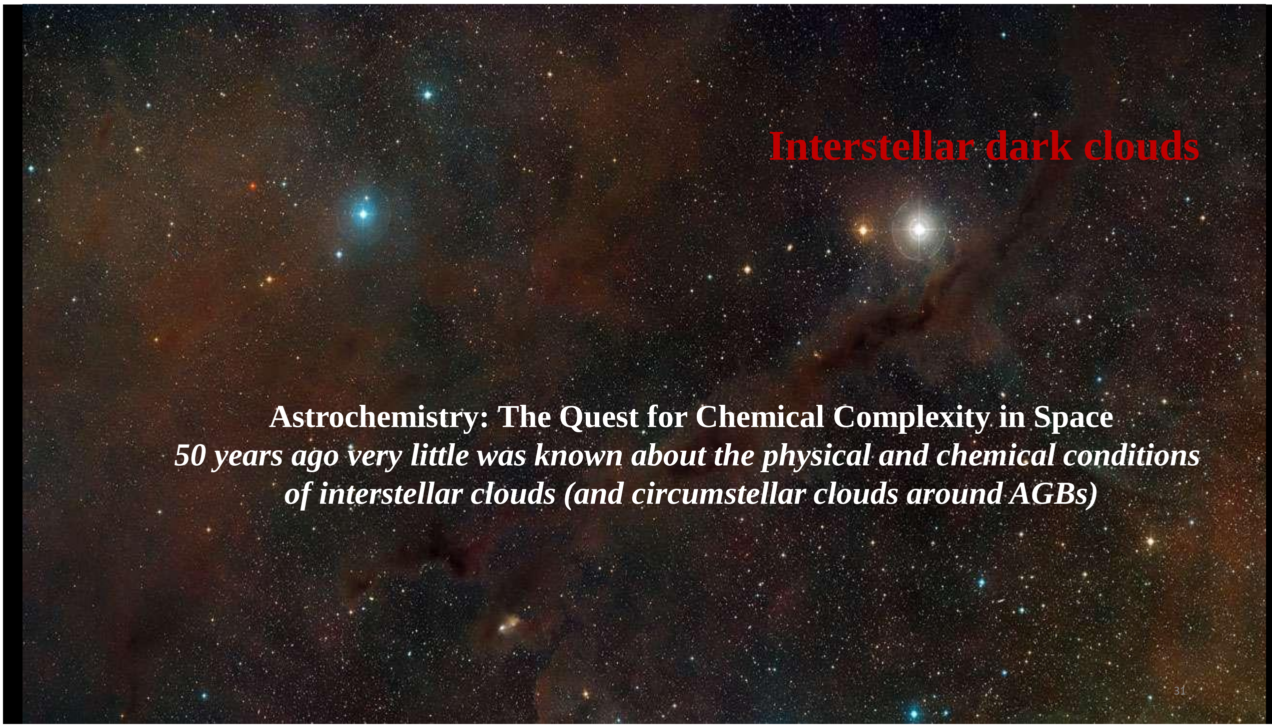
Interstellar dark clouds
Astrochemistry: The Quest for Chemical Complexity in Space
50 years ago very little was known about the physical and chemical conditions
of interstellar clouds (and circumstellar clouds around AGBs)
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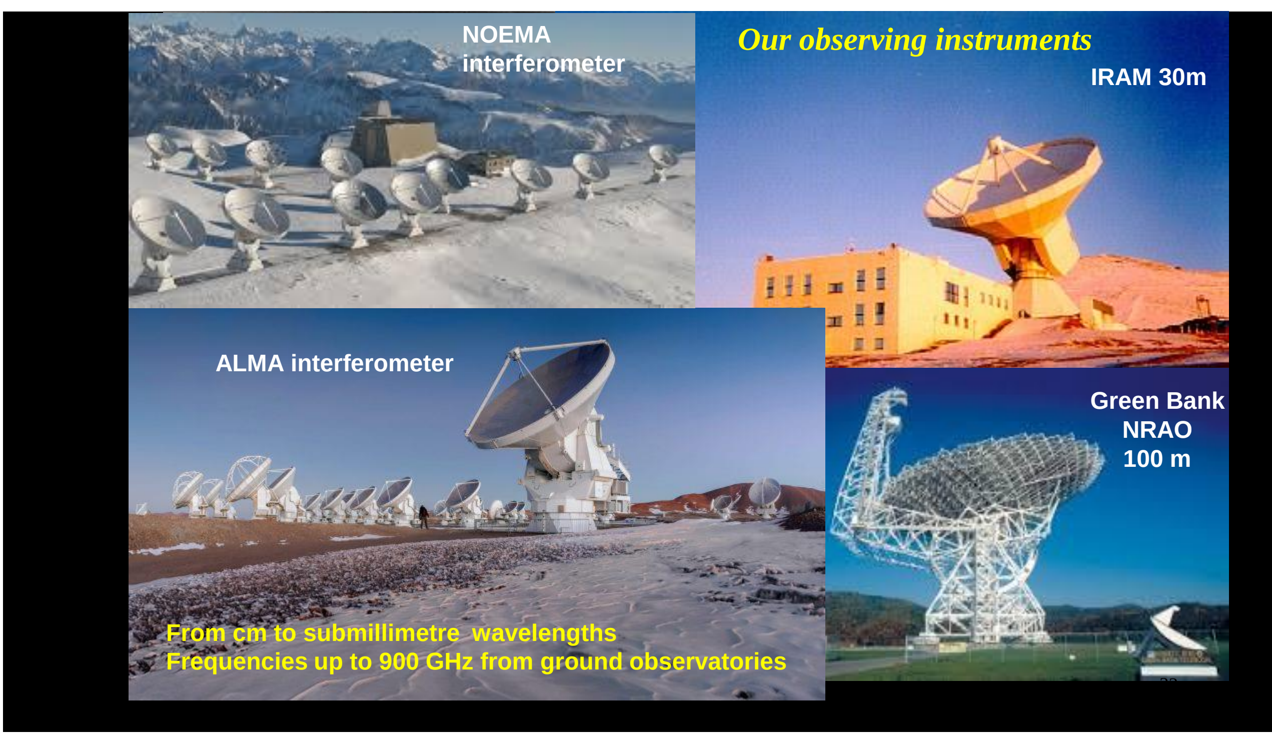
NOEMA
interferometer
Our observing instruments
IRAM 30m
ALMA interferometer
Green Bank
NRAO
100 m
From cm to submillimetre wavelengths
Frequencies up to 900 GHz from ground observatories

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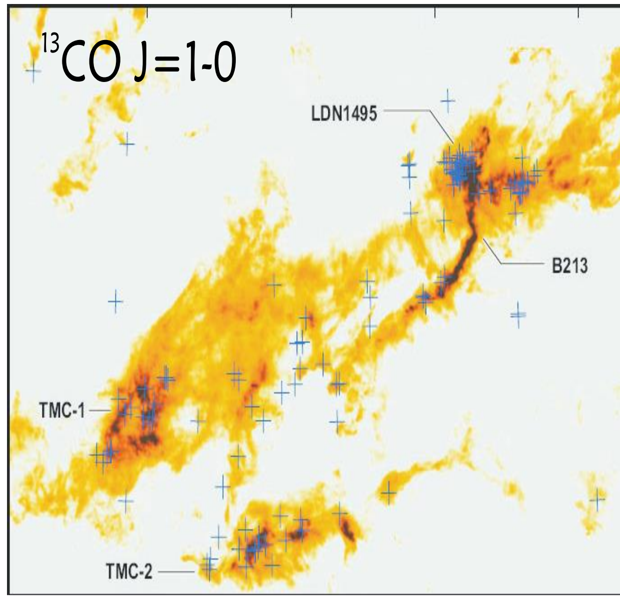

Dark clouds in the Taurus complex at visible wavelength (left; Barnard 1919) and in the emission of 13CO J=1-0 (pictures from Bergin and Tafalla 2007, ARAA, 45 339; ^{13}CO data from Goldsmith et al. 2008, ApJ, 680, 428). 33

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First detailed proposal to search for atoms and molecules in space

PAPER 16

MICROWAVE AND RADIO-FREQUENCY RESONANCE LINES OF INTEREST TO RADIO ASTRONOMY

C.H. Townes, 1957, IAU Symposium, Vol 4, pages 92-103

(67 years ago)

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Table 3

Some microwave transitions between molecular rotational levels of interest to radio astronomy. The inversion spectrum of NH_3 is also listed.

Molecule	Electronic state	Transition	Frequency (Mc./s.)	Matrix element in Debye units	Comments
CaH	$^2\Sigma$	$J=3/2-1/2$ $J=1/2-1/2$	254,080 252,650	Electric dipole unknown	
CO	$^1\Sigma$	$J=1-0$	115,270·6	0·10	
CO^+	$^2\Sigma$	$J=3/2-1/2$, $1/2-1/2$	117,980	Electric dipole unknown	
CS	$^1\Sigma$	$J=1-0$	48,991·0	2·0	
NO	$^2\Pi_{1/2}$	$J=3/1-1/2$	150,176·3	0·07	Also other nearby lines due to h.f.s.
H_2O	$^1\Sigma$	$6_{1,6}-5_{2,3}$	22,235·22	0·16	
N_2O	$^1\Sigma$	$J=1-0$	25,123·28	0·17	Other lines at multiples of the frequency given. Very small h.f.s. present
HCN	$^1\Sigma$	$J=1-0$, $F=1-1$ $F=2-1$ $F=0-1$	88,600·1 88,601·5 88,603·6	1·72 2·22 0·99	Also l-doublet transitions may occur
CH_2					Structure and spectrum unknown, but may produce some microwave lines
NH_2					Structure and spectrum not well known, but probably produces some microwave lines
NH_3	$^1\Sigma$	Inversion, $J=1$, $K=1$	23,694·48	1·0	Also other inversion transitions at nearby frequencies
O_3	$^1\Sigma$	$1_{11}-2_{02}$ $1_{11}-0_{00}$	42,832·62 118,364·3	0·17 0·53	Also other rotational transitions

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First molecules detected in space

optical and centimeter wavelengths

- **CN, CH and CH^+ detected between 1930-1940 through optical observations**
- **In 1957 C. Townes proposed that some molecules could be present in the ISM**
- **NH_3 detected in 1968 using a Dicke radiometer (Tsys=2000 K) mounted on the 20ft diameter dish of Hat Creek (U. California) by Cheung, Rank, Townes, Thornton and Welch (PRL, 21, 1701)**
- **H_2O detected in 1969 towards W49 with the Hat Creek radio telescope by Cheung, Rank, Townes, Thornton & Welch (Nature, 221, 626)**
- **H_2CO detected in 1969 by Snyder, Buhl, Zuckerman and Palmer (PRL, 22, 679) using the 140ft Green Bank telescope**

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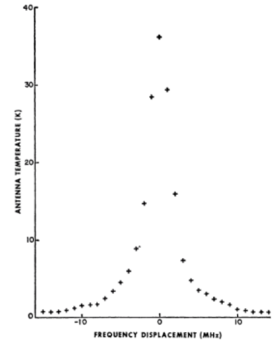
The discovery of CO and Millimeter Radio Astronomy. The birth of Astrochemistry

THE ASTROPHYSICAL JOURNAL, 161:L43–L44, July 1970

CARBON MONOXIDE IN THE ORION NEBULA

R. W. WILSON, K. B. JEFFERTS, AND A. A. PENZIAS
Bell Telephone Laboratories, Inc., Holmdel, New Jersey, and
Crawford Hill Laboratory, Murray Hill, New Jersey
Received 1970 June 5

ABSTRACT
We have found intense 2.6-mm line radiation from nine galactic sources which we attribute to carbon monoxide.



This work was done with a specially constructed line receiver mounted on the NRAO 36′ paraboloid. Schottky barrier diodes developed by C. A. Burrus of Bell Laboratories were used in Sharpless wafer units both in the signal mixer and in a harmonic mixer used to control the frequency of the local oscillator klystron.

Seven molecules discovered between 1936-1970 : CN, CH, CH^+, NH_3, H_2O, H_2CO, CO 37

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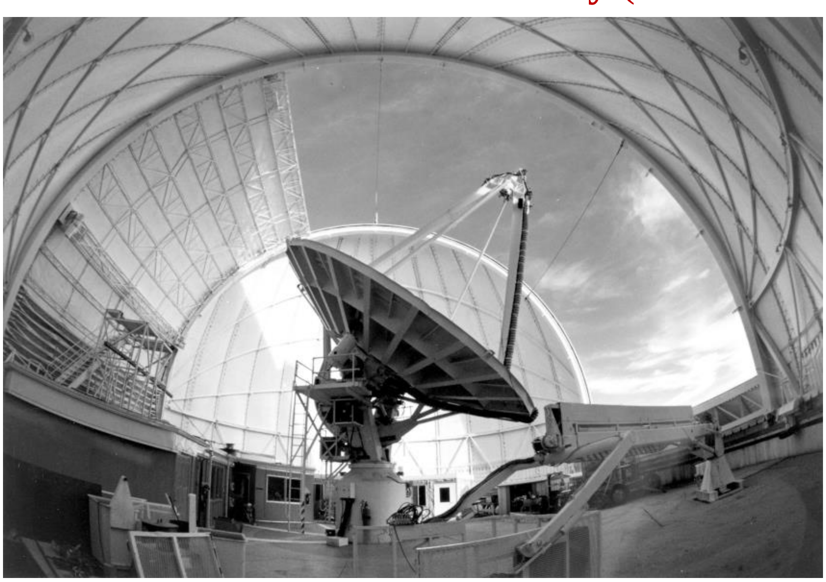
Kitt Peak 12m radio telescope (NRAO) Millimeter Radio Astronomy (around 30 molecules detected)



Before CO detection only six molecules were known in space (1936-1970)

By 1980 around 50 molecules (around 30 of them with the Kitt Peak radio telescope)

Between 1980 and Sep 2020 around 200 molecules (mainly with the IRAM 30m, Nobeyama 45 m, and Green Bank 100m telescopes)

By April 2024 around 310 molecules found in space (mainly through GOTHAM and QUIJOTE line surveys). In four years the number of detected molecular species in space has increased by a factor 1.5

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2 atoms

CH	SO^+
CN	CO^+
CH^+	HF
OH	N_2
CO	CF^+
H_2	PO
SiO	O_2
CS	AlO
SO	CN^-
SiS	OH^+
NS	SH^+
C_2	HCl^+
NO	SH
HCl	TiO
$NaCl$	ArH^+
$AlCl$	NS^+
KCl	HeH^+
AlF	VO
PN	*FeO*
SiC	*SiH*
CP	*NO^+*
NH	PO^+
SiN	SiP

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3 atoms

H_2O	$MgCN$
HCO^+	H_3^+
HCN	$SiCN$
OCS	$AlNC$
HNC	$SiNC$
H_2S	HCP
N_2H^+	CCP
C_2H	$AlOH$
SO_2	H_2O^+
HCO	H_2Cl^+
HNO	KCN
HCS^+	$FeCN$
HOC^+	HO_2
SiC_2	TiO_2
C_2S	CCN
C_3	$SiCSi$
CO_2	S_2H
CH_2	HCS
C_2O	HSC
$MgNC$	NCO
NH_2	$CaNC$
$NaCN$	NCS
N_2O	MgC_2

46

4 atoms

NH_3	CH_3
H_2CO	C_3N^-
$HNCO$	PH_3
H_2CS	$HCNO$
C_2H_2	$HOCN$
C_3N	$HSCN$
$HNCS$	$HOOH$
$HOCO^+$	l-C_3H^+
C_3O	$HMgNC$
l-C_3H	$HCCO$
$HCNH^+$	$CNCN$
H_3O^+	$HONO$
C_3S	$MgCCH$
c-C_3H	$HCCS$
HC_2N	$HNCN$
H_2CN	H_2NC
SiC_3	HC_2S^+

34

5 atoms

HC_3N	$HNCNH$
$HCOOH$	CH_3O
CH_2NH	NH_4^+
NH_2CN	H_2NCO^+
H_2CCO	$NCCNH^+$
C_4H	CH_3Cl
SiH_4	MgC_3N
c-C_3H_2	HC_3O^+
CH_2CN	NH_2OH
C_5	HC_3S^+
SiC_4	H_2CCS
H_2CCC	C_4S
CH_4	$CHOSH$
$HCCNC$	$CHSCN$
$HNCCC$	HC_3O
H_2COH^+	NaC_3N
C_4H^-	MgC_3N^+
$CNCHO$	

35

6 atoms

CH_3OH	C_5N^-
CH_3CN	$HNCHCN$
NH_2CHO	SiH_3CN
CH_3SH	MgC_4H
C_2H_4	CH_3CO^+
C_5H	H_2CCCS
CH_3NC	CH_2CCH
HC_2CHO	$HCSCCH$
H_2C_4	C_5O
C_5S	C_5H^+
HC_3NH^+	$HCCNCH^+$
C_5N	c-C_5H
HC_4H	HC_4S
HC_4N	$HMgC_3N$
c-H_2C_3O	MgC_4H^+
CH_2CNH	

31

7 atoms

CH_3CHO, CH_3CCH, CH_3NH_2, CH_2CHCN, HC_5N, C_6H, c-C_2H_4O, CH_2CHOH, C_6H^-, CH_3NCO, HC_5O, $HOCH_2CN$, HC_4NC, HC_3HNH, c-C_3HCCH, H_2C_5, MgC_5N, CH_2C_3N, NC_4NH+, MgC_5N+

20

8 atoms

$HCOOCH_3$, CH_3C_3N, C_7H, CH_3COOH, H_2C_6, CH_2OHCHO, HC_6H, CH_2CHCHO, CH_2CCHCN, NH_2CH_2CN, CH_3CHNH, CH_3SiH_3, NH_2CONH_2, $HCCCH_2CN$, CH_2CHCCH, HC_5NH^+, MgC_6H, $C_2H_3NH_2$, $(CHOH)_2$, $HCCCHCCC$, C_7N^-, CH_3CHCO, MgC_6H^+

23

9 atoms

CH_3OCH_3, CH_3CH_2OH, CH_3CH_2CN, HC_7N, CH_3C_4H, C_8H, CH_3CONH_2, C_8H^-, CH_2CHCH_3, CH_3CH_2SH, HC_7O, CH_3NHCHO, $H_2CCCHCCH$, $HCCCHCHCN$, H_2CCHC_3N, *$HOCHCHOH$*, *$CH_2CHCHNH$*

17

10 atoms

CH_3COCH_3, $HOCH_2CH_2OH$, CH_3CH_2CHO, CH_3C_5N, CH_3CHCH_2O, CH_3OCH_2OH, c-C_6H_4, CH_2CCHC_3N, C_2H_5NCO, *$C_2H_5NH_2$*, HC_7NH^+, $CH_3CHCHCN$, CH_3CCNCH_2, CH_2CHCH_2CN

14

11 atoms

HC_9N, CH_3C_6H, C_2H_5OCHO, CH_3COOCH_3, CH_3COCH_2OH, c-C_5H_6, $HOCH_2CH_2NH_2$, CH_2CCHC_4H, $C_{10}H^-$, 1-C_4H_5CN

10

12 atoms

c-C_6H_6, n-C_3H_7CN, i-C_3H_7CN, 1-C_5H_5CN, 2-C_5H_5CN, $C_2H_5OCH_3$, CH_3C_7N, n-C_3H_7OH, i-C_3H_7OH

9

13 atoms

c-C_6H_5CN, $HC_{11}N$

2

PAHs

1-$C_{10}H_7CN$, 2-$C_{10}H_7CN$, C_9H_8

3++

fullerenes

C_{60}, C_{60}^+, C_{70}

3

Blue molecules = at least one carbon atom

Source: CDMS (April 2023)

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Molecules as tracers of the physical conditions of molecular clouds

Rotational levels are out of equilibrium. Hence, the observation of several rotational lines of a molecule permits to derive volume densities, kinetic temperatures and molecular abundances.

The high spectral resolution (cm/s) achieved in radio astronomy allows the study of the kinematics and the dynamical state of interstellar clouds

The high angular resolution provided by interferometers such as VLA, ALMA, and NOEMA permits to study protoplanetary discs around newly formed stars and the dust formation zone around evolved stars.

Infrared observations with ISO, Spitzer, Herschel and now JWST, permit the observation and study of light species (OH, CH, CH^+, H_2O, NH_3, H_2O^+, H_3O^+,..) and of species without permanent dipole moment (H_2, CH_4, C_2H_2, C_2H_4, C_4H_2, C_6H_2, C_6H_6,…).
See, e.g., the recent detection with the JWST of CH_3^+ towards a proplyde in Orion (Berné et al., 2023, Nature)

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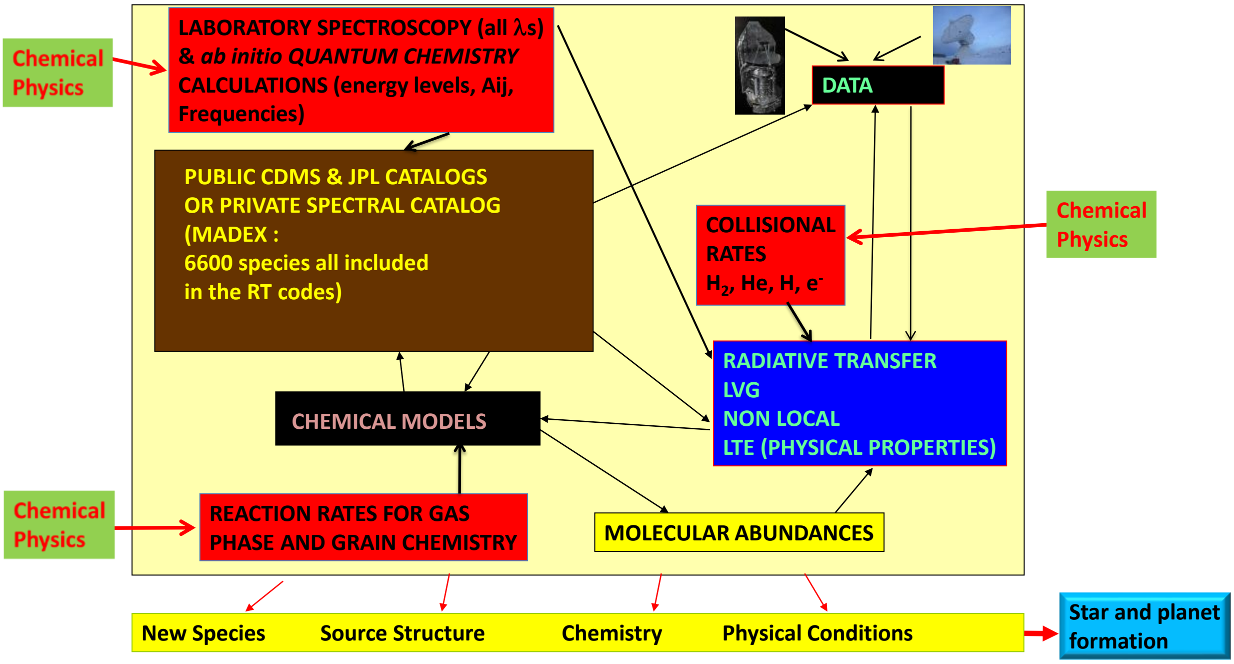
ASTROCHEMISTRY AS A MULTISDICIPLINARY FIELD



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Laboratory Astrophysics has played a key role in the last 50 years in the development of astrochemistry:

- **Low temperature measurements of reaction rates** (CRESU machines)
  Cinétique de Réaction en Ecoulement Supersonique Uniforme = Reaction kinetics in uniform supersonic flow also ion traps for cations and anions
- **Rotational and infrared spectroscopy of unstable species** (radicals, cations, and anions)
- **Studies of ices : chemical reactivity, spectroscopy, studies of the formation of molecules**
- **State-to-state collisional rates of molecules with H_2, He, e^- and other species**
- **Quantum chemical structural calculations of a large sample of possible candidates for a pattern of lines with unknown carrier in a given line survey**
- **Very precise quantum chemical ab initio calculations when exotic molecules can not be produced in the laboratory**
- **PAH studies** (reactivity, spectroscopy, ionization, photodissociation…)

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LINE SURVEYS

THE QUEST FOR MOLECULAR COMPLEXITY

THE NEED OF SENSITIVITY, INSTANTANEOUS BANDWIDTH

FREQUENCY COVERAGE

AND ANGULAR RESOLUTION

IMPRESSIVE IMPROVEMENTS IN RECEIVER TECHNOLOGIES, SENSITIVITY, INSTANTANEOUS BANDWIDTH AND BACKEND FREQUENCY COVERAGE IN THE LAST 50 years

What is done nowadays in 24 hours would require several years of observing time 50 years ago

factor >100 in frequency coverage (number of frequency setups)
factor > 1000 in time due to $t \propto T_{sys}^2$

43

Some sensitive line surveys achieved with high spectral resolution

- Sgr B2 (Belloche et al. 2008, A&A, 482, 179) 3mm and 2mm
- Sgr B2 –PRIMOS- (Neill et al. 2012, ApJ, 755, 153) up to 50 GHz
- IRC+10216 (2mm, Cernicharo et al. 2000, A&A SS, 142, 181)
- Orion Bar (mm; Cuadrado et al. 2015, A&A, 575,A82)
- IRAS16923-2422 ALMA-PILS (Jorgensen et al. 2016, A&A, 595, A117) 0.8 mm
- Orion KL (Tercero et al. 2010, A&A, 517, A96) 3, 2 and 1mm (spectral confusion limited)
- G+0.693-0.027 (Rivilla et al. 2022, ApJ, 929, L11; Jiménez-Serra et al. 2022, A&A, 663, A181)
- HEXOS (Herschel/HIFI), several sources, Bergin et al. 2010, A&A, 521, L20 (0.5-2 THz)
- CHESS (Herschel/HIFI), several sources, Ceccarelli et al. 2010, A&A, 521, L22 (0.5-2 THz)
- IRC+10216 in the infrared (Fonfría et al. 2008, ApJ. 673, 445) 11-14 µm
  TEXES and EXES/SOFIA instruments ($\lambda/\Delta\lambda \approx 75000$)
- TMC-1 (GOTHAM & QUIJOTE)
- G+0693-0.027 (V. Rivilla, I. Jiménez, et al., 2023, ApJ, 953, L20

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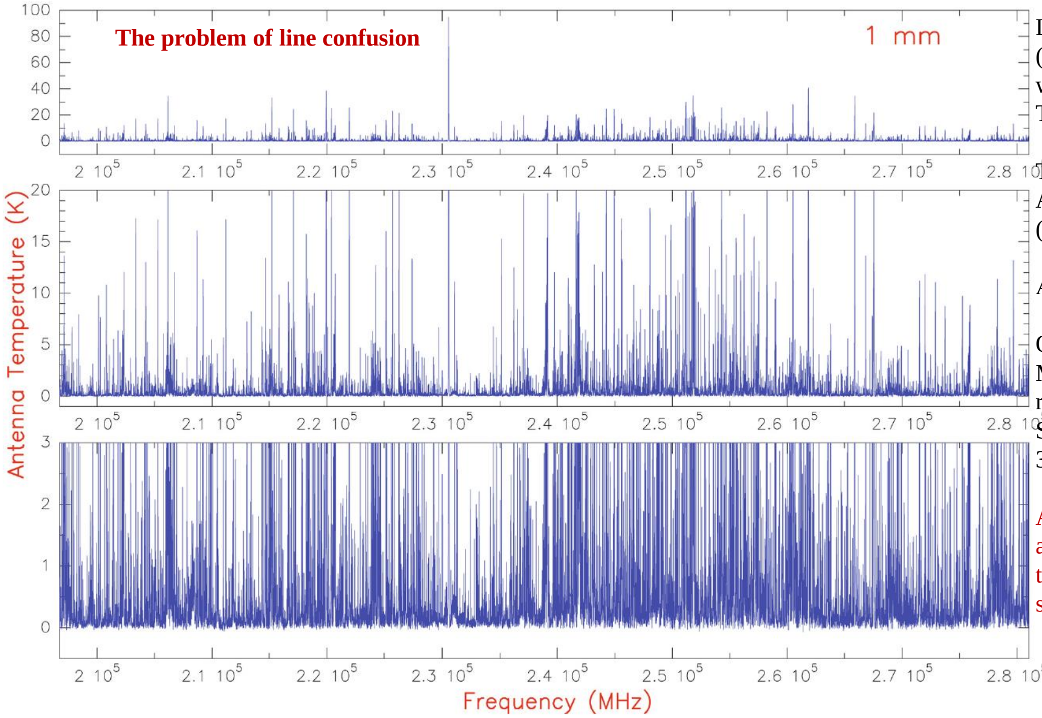

Line survey of Orion KL (T_K=150K) at 1.3mm with the IRAM 30m Telescope

Tercero et al 2010, A&A, 517, A96 (3, 2 and 1.3 mm)

Angular resolution=10"

Orion is a warm high Mass star forming region. There are many Sources inside the IRAM 30m beam

ALMA observations are needed to separate the emission from each source

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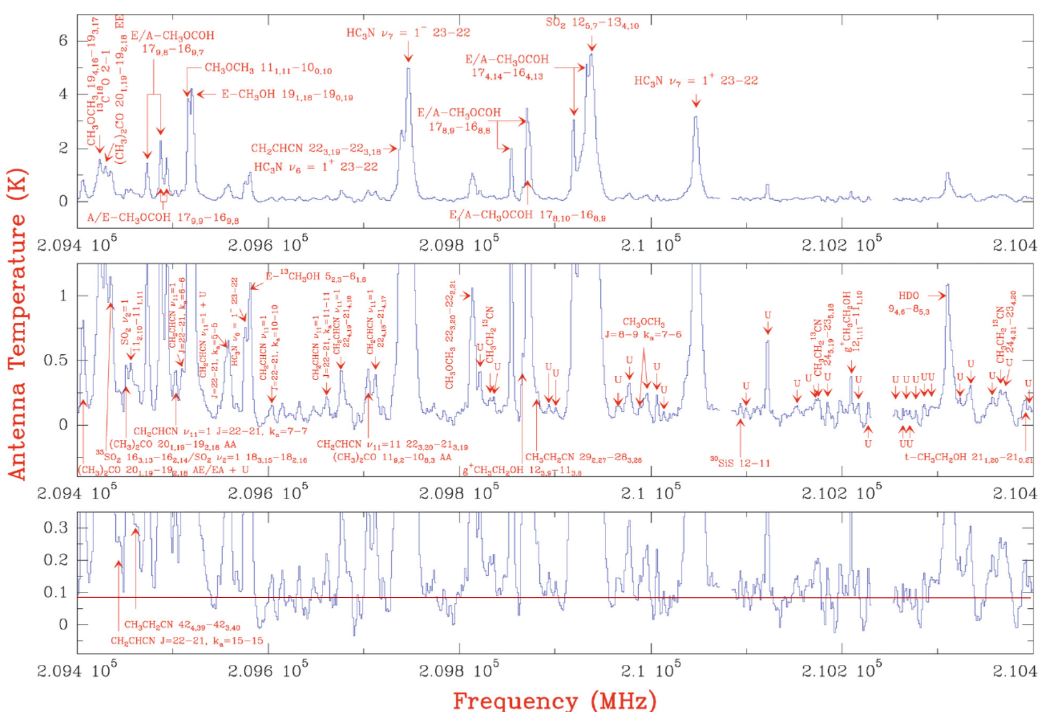

At 1.3 mm (230 GHz) the confusion limit is reached

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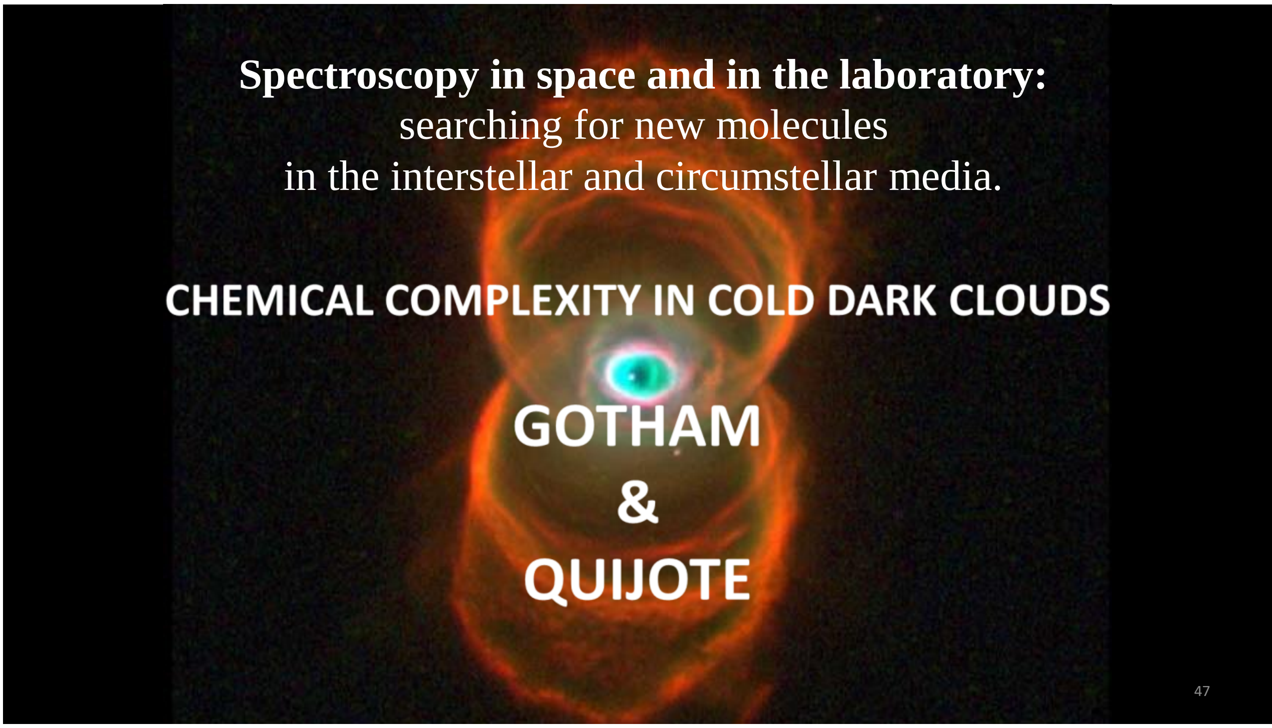

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GOTHAM line survey of TMC-1 (a cold dark cloud in Taurus)

- Green Bank 100 m telescope observations 1-50 GHz (cm wavelengths)
- Most molecules detected through statistical analysis of the noise trough spectral stacking. Very powerful technique !!!
- Discovery of CN derivatives of PAHs in a cold dark cloud
- C_6H_5CN (benzonitrile) and $C_{10}H_7CN$ (cyano-naphthalene, 2 isomers)
- Several cyanide derivatives of hydrocarbons; indene
- McGuire et al. 2018, Science, 359, 202
- McGuire et al. 2021, Science, 371, 1265
- How, and where, these PAHs are formed?

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QUIJOTE: The limits of sensitivity

- Building new and novel ultrasensitive broadband receivers for the Yebes 40m radio telescope (NANOCOSMOS)

- Exploring the sub milli Kelvin chemical work
- Reaching unexplored limits of sensitivity
- To see what radio astronomers have never seen before !
- To identify molecules through classical techniques of line by line detection
- SANCHO: Fidel companion of QUIJOTE. High sensitivity maps of the molecular emission at the milli Kelvin level.

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The Yebes observatory is located in the region of La Mancha, the land of Don Quixote, at 950 m of altitude. It is around 60 km away from Madrid

The radio telescope was built and equipped for VLBI observations

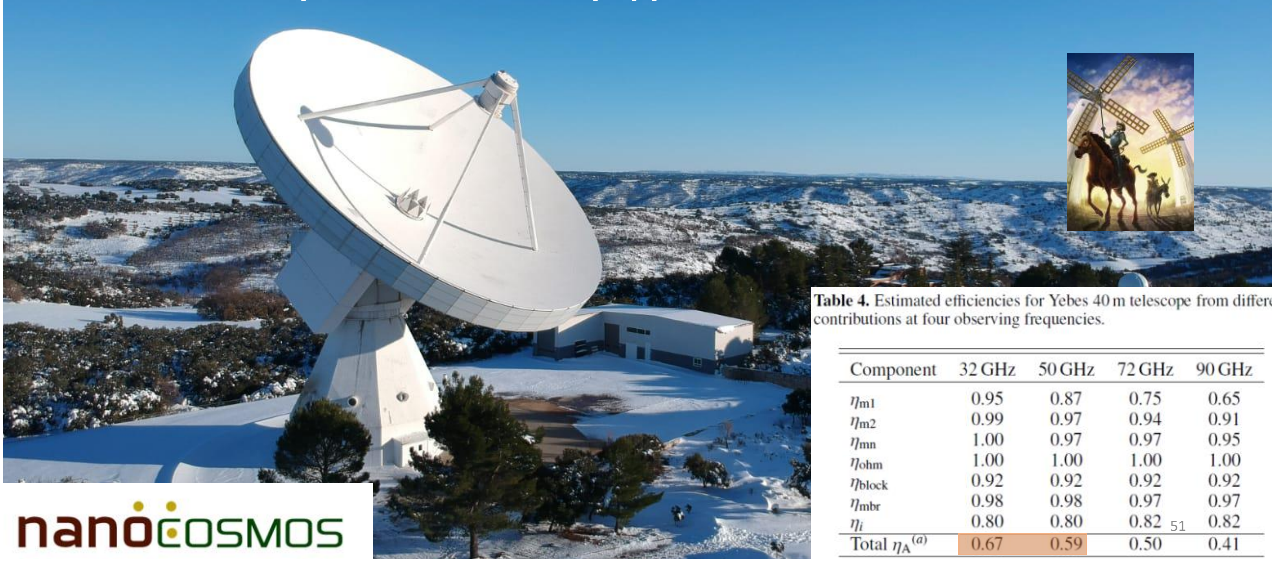

Table 4. Estimated efficiencies for Yebes 40 m telescope from differen contributions at four observing frequencies.

Component	32 GHz	50 GHz	72 GHz	90 GHz
η_{m1}	0.95	0.87	0.75	0.65
η_{m2}	0.99	0.97	0.94	0.91
η_{mn}	1.00	0.97	0.97	0.95
η_{ohm}	1.00	1.00	1.00	1.00
η_{block}	0.92	0.92	0.92	0.92
η_{mbr}	0.98	0.98	0.97	0.97
η_{i}	0.80	0.80	0.82	0.82
Total η_A [(a)]	0.67	0.59	0.50	0.41

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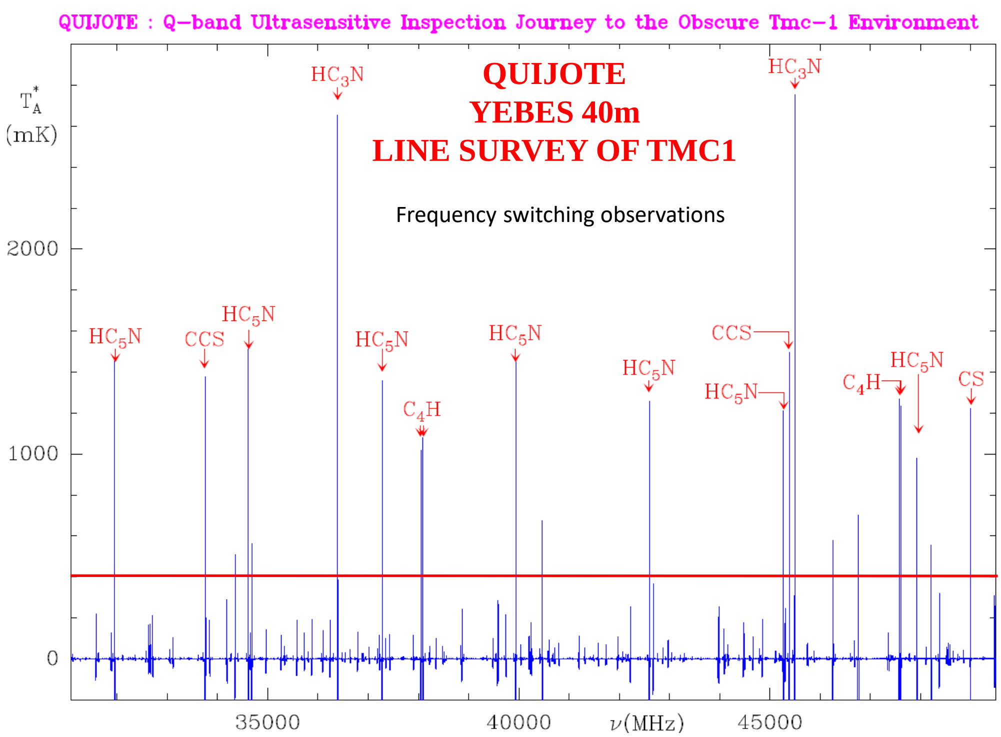

only 22 lines above 400mK

A few more above 200 mK

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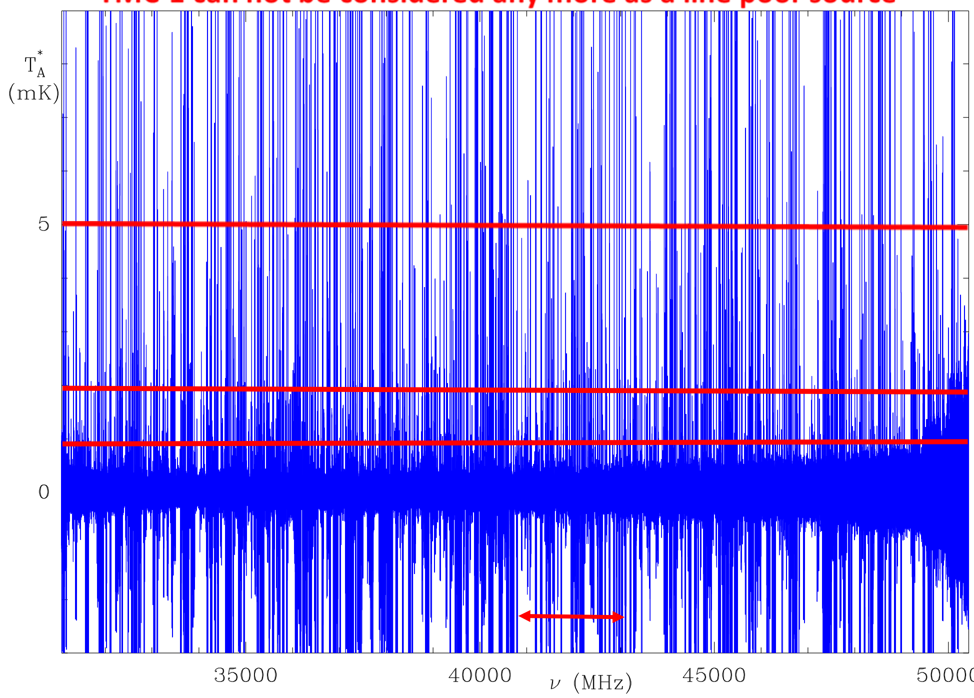
TMC-1 can not be considered any more as a line poor source



Between 5-50 mK several new species

Below 5 mK:
A forest of lines from isotopologues and unknown species

2 mK

1 mK

Data by Sept 2023

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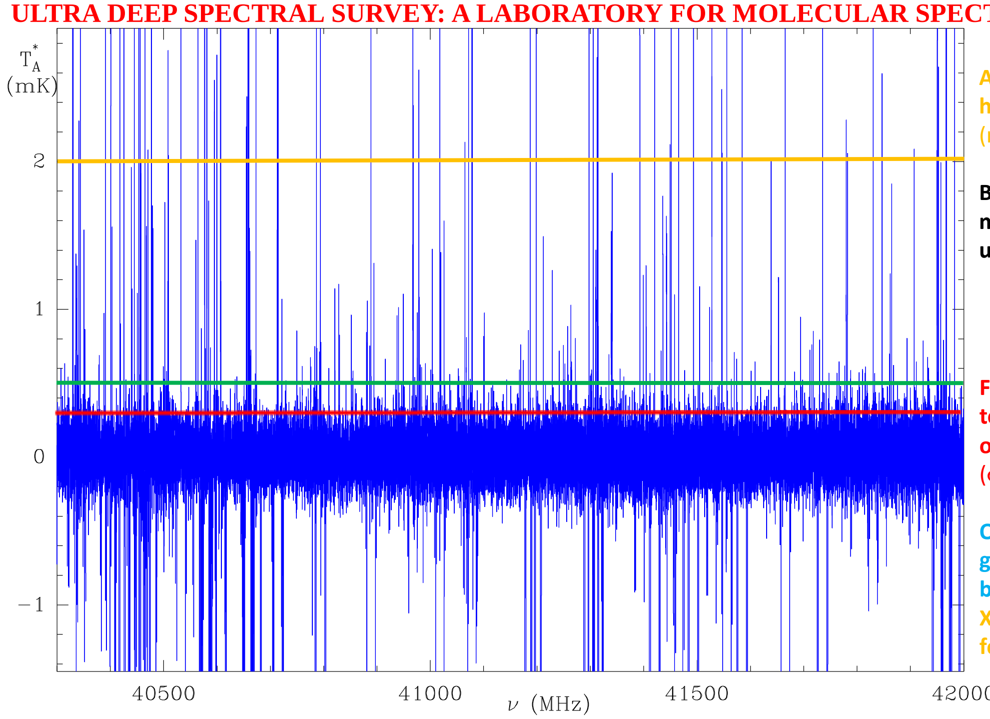
ULTRA DEEP SPECTRAL SURVEY: A LABORATORY FOR MOLECULAR SPECTROSCOPY



Above 2 mK most lines have been assigned
(many new molecules)

Below 2 mK most lines are unidentified

Sensitivity by Sept. 2023 of 0.5 mK (5σ)

FINAL GOAL to detect lines of 0.30 mK at 5σ
(σ=0.06 mK)

On-going project; goal to be reached by 2024/2025

X > 10^{-12} for very polar species

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Data analysis and data interpretation

- **Data analysis:** very tedious data analysis procedure with 2560 spectral windows per run (x 19 runs x 2 polarizations). Always performed by JC to keep homogeneity of the data products. Each run takes near one month of work.

- **Data interpretation:** Use of the best spectral catalogues (CDMS and JPL) is not enough to interpret the data and to get the molecular content included in QUIJOTE.

- **MADEX Catalogue:** 6600 spectral entries with laboratory information. Maintained by JC since 1985. Automatic identification of the molecules in QUIJOTE using a simple assignment code and automatic identification of unknown spectral features (U-lines).

- **Elaborated analysis of spectral patterns within the U-features.** TMC-1 as a laboratory for molecular spectroscopy.

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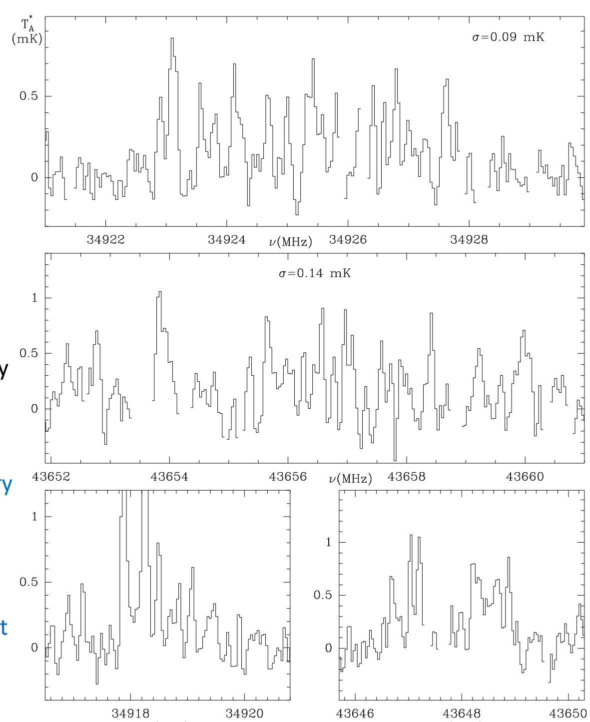
SPECTRAL PURITY

TMC-1 can not be considered as a poor line source at the QUIJOTE's sub mK level

Looking for specific spectroscopic patterns it is possible to discover new molecular species without any previous information on the frequencies.

TMC-1 is a chemical laboratory for molecular spectroscopy thanks to QUIJOTE and NANOCOSMOS.

QUIJOTE can now fight against the giant windmills of the forest of U-lines of TMC-1



ν_2/ν_1=1.249993 ≈ 5/4

Transitions J=5-4 and J=4-3 of a new radical ???

B or (B+C)/2 ≈ 4365 MHz

HCCCN has B=4549.1 MHz

H_2CCCN ???

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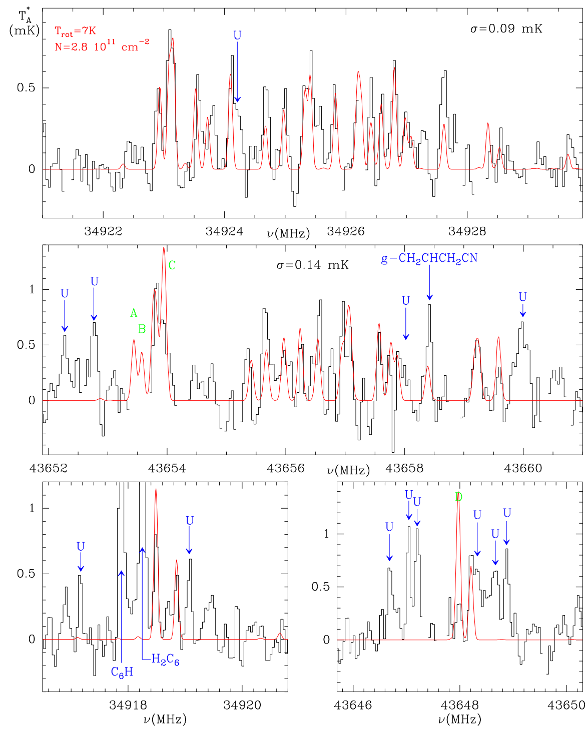
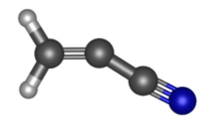


Excellent data quality
All features are real.
Sensitivity continues to increase with time.

Systematic instrumental effects removed and understood



H_2CCCN radical
Cabezas et al. 2023, A&A, 676, L5

Laboratory data from Endo's team

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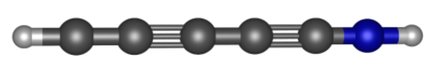
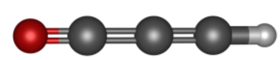
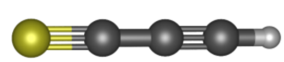
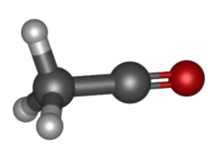
TMC-1 as a spectroscopic laboratory

- **Detection of species WITHOUT previous laboratory data**. Searching for systematic spectral patterns in the data. Confirming assignments in the laboratory when possible and through ab initio calculations
- **HC_5NH^+** Marcelino et al., 2020, A&A, 643, L6
- **HC_3O^+** * Cernicharo et al., 2020, A&A, 642, L17
- **HC_3S^+** * Cernicharo et al., 2021, A&A, 646, L3
- **CH_3CO^+** * Cernicharo et al., 2021, A&A, 646, L7
- **C_5H^+** Cernicharo et al., 2022, A&A, 657, L16
- **HC_7NH^+** Cabezas et al., 2022, A&A, 659, L8
- **$HCCNCH^+$** Agúndez et al., 2022, A&A, 659, L9
- **$HCCS^+$** Cabezas et al., 2022, A&A, 657, L4
- **C_7N^-** Cernicharo et al. 2023, A&A, 670, L19
- **NC_4NH^+** Agúndez et al. 2023, A&A, 669, L1
- **$C_{10}H^-$** GOTHAM, Remijan et al. 2023, ApJ, 944, L45 (also in IRC+10216; Pardo et al. 2023,A&A, 677, A55)
- **And isotopologues such as HDCCN, Cabezas et al., 2021, A&A, 646, L1; CH_2DC_3N, Cabezas et al, 2021**
- Additionally, QUIJOTE has confirmed the previous detection of C_5N^- in IRC+10216 by detection of six narrow lines of this species in TMC-1 (**together with C_3N^-**). Rotational constants for these species have been improved.









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A&A 657, L4 (2022)
https://doi.org/10.1051/0004-6361/202142815

LETTER TO THE EDITOR

Discovery of the elusive thioketenylium, HCCS+, in TMC-1

C. Cabezas[1], M. Agúndez[1], N. Marcelino[2,3], B. Tercero[2,3], Y. Endo[4], R. Fuentetaja[1], J. R. Pa
P. de Vicente[3], and J. Cernicharo[1]

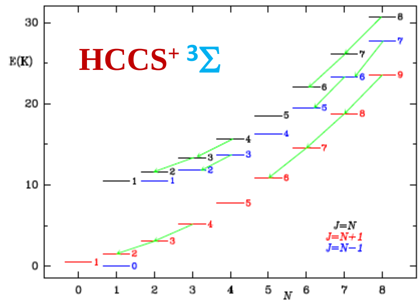
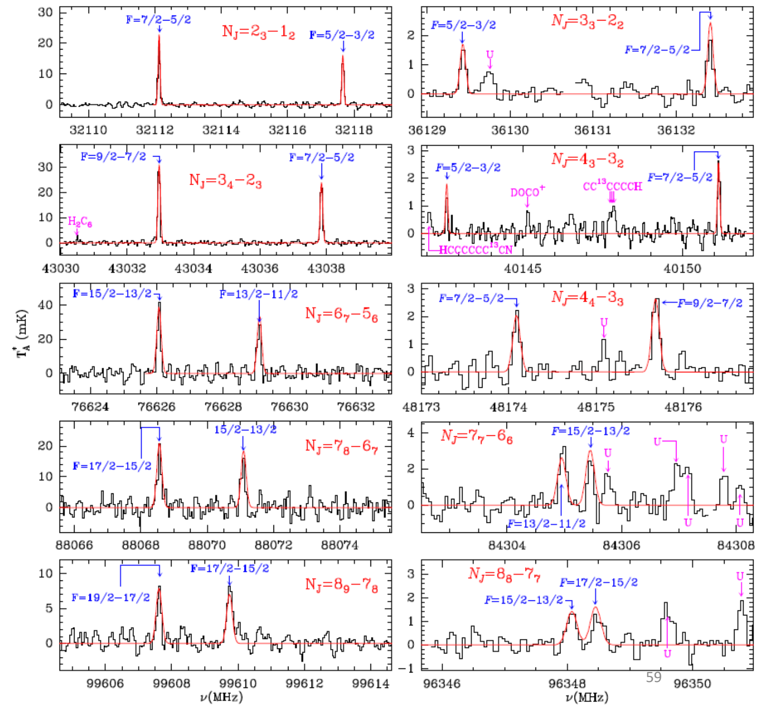


Table 1. Spectroscopic parameters of $HCCS^+$, in MHz.

Parameter	TMC-1 fit	Theoretical	CCS [a]
B	6021.89878(55) [b]	6021.2 [c],[d]	6477.75036(71)
D	0.0012543(72)	0.00120 [e]	0.00172796(95)
λ	108970.78(83)	–	97196.07(77)
λ_D	0.04060(65)	–	0.02700(67)
γ	−41.776(46)	−18.4 [e]	−14.737(49)
$b_F^{(H)}$	−44.961(23)	−47.6 [f]	–
$c^{(H)}$	31.663(70)	71.6 [f]	–
σ [g]	26.1	–	18
N	26	–	31



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$HCC^{34}S^+$

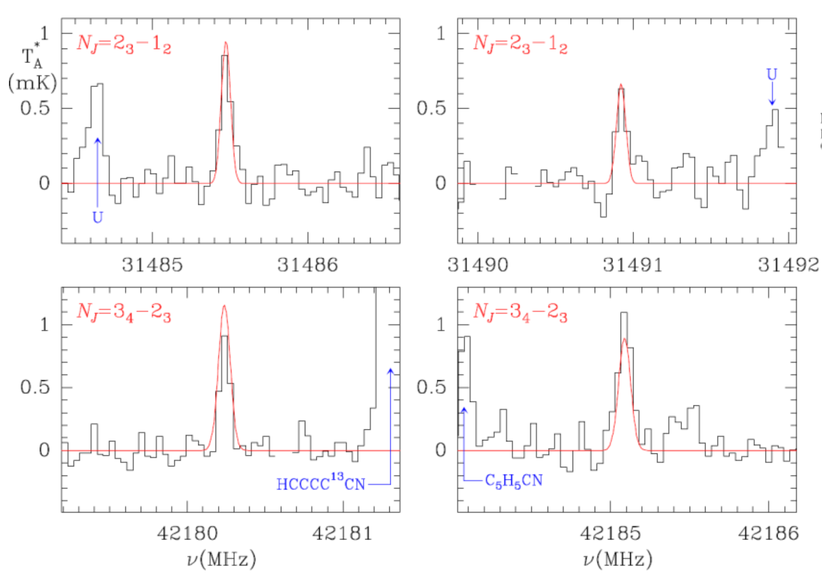

Table A.8. Spectroscopic parameters of $HCC^{34}S^+$

Parameter	$HCC^{34}S^+$
B (MHz)	5889.02214(82) [a]
D (KHz)	[1.2543] [b]
λ (MHz)	[108970.78] [b]
λ_D (kHz)	[40.60] [b]
γ (MHz)	[−41.776] [b]
$b_F^{(H)}$ (MHz)	−45.024(99)
$c^{(H)}$ (MHz)	[31.663] [b]
σ (kHz)	8.0
N_{lines}	4

Notes. [a] Numbers in parentheses are 1σ uncertainties in units of the last digits.
[b] Fixed to the value reported by Cabezas et al. (2022a) for $HCCS^+$.

Fuentetaja et al. 2024, in prep.

$HCCS^+$ fully confirmed from space data

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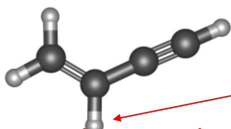
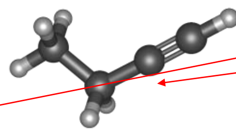
Pure hydrocarbons in TMC-1

arXiv:2106.00635

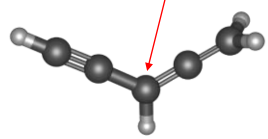
- **Discovery of several high abundant pure hydrocarbons, including three cycles (species with low dipole moment)**

- **CH_2CHCCH**, Cernicharo et al. 2021, A&A, 647, L2 (together with HCCN, HC_4N, CH_3CH_2CN and tentatively CH_3CH_2CCH)

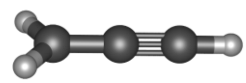


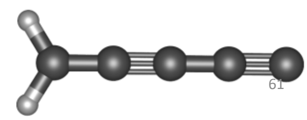


Very abundant species



- **$H_2CCCHCCH$,** Cernicharo et al. 2021, A&A, 647, L3
- **$H_2CCCHCCCH$**, Fuentetaja et al. 2022, A&A, 663, L3
- **HCCCHCCC,** Fuentetaja et al., 2022, 667, L4
- **H_2CCCH,** Agúndez et al., 2021, 647, L10 **(extremely abundant !!!)**
- **c-C_5H,** Cabezas et al. 2022, A&A, 663, L2
- **H_2C_5,** Cabezas et al., 2021, A&A, 650, L9





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A&A 649, L15 (2021)
https://doi.org/10.1051/0004-6361/202141156

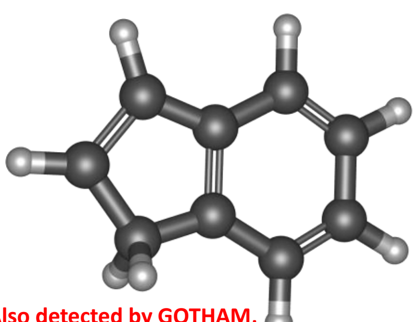
Astronomy & Astrophysics

LETTER TO THE EDITOR

Pure hydrocarbon cycles in TMC-1: Discovery of ethynyl cyclopropenylidene, cyclopentadiene, and indene★

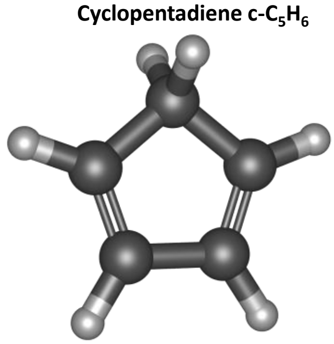
J. Cernicharo[1], M. Agúndez[1], C. Cabezas[1], B. Tercero[2,3], N. Marcelino[1], J. R. Pardo[1], and P. de Vicente[2]

Indene c-C_9H_8

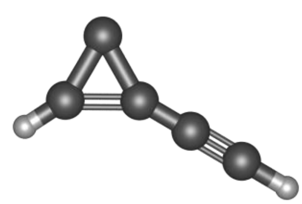


Also detected by GOTHAM, Burkhardt et al. 2021, ApJ, 913, L18

Cyclopentadiene c-C_5H_6



CN derivatives of cyclopentadiene detected by GOTHAM



Ethynyl cyclopropenylidene c-C_5H_2

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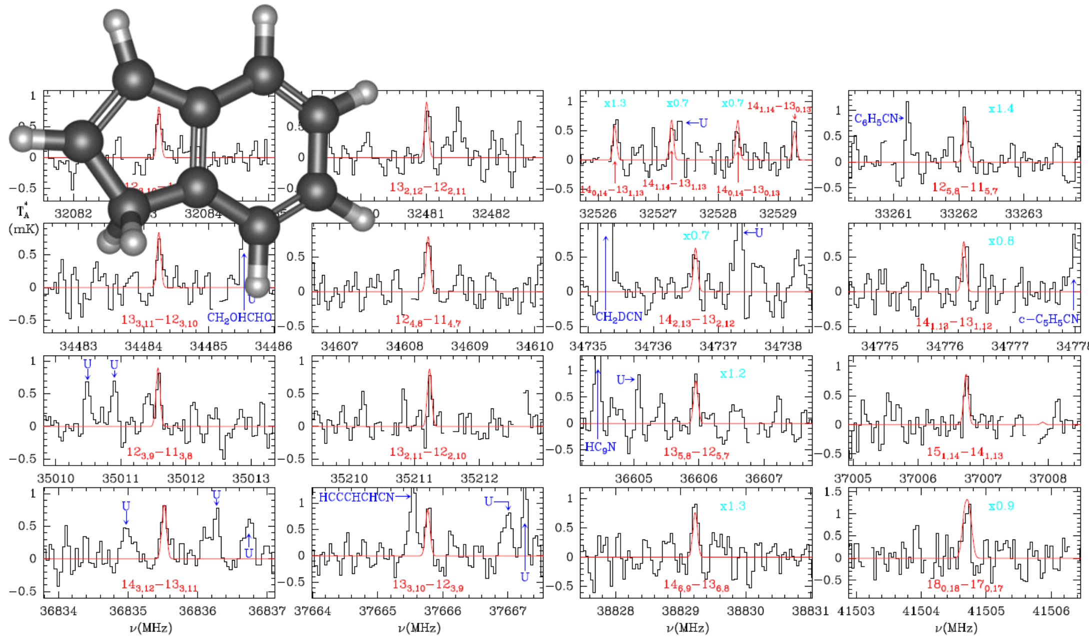

Fig. 4. Same as Fig. 2 but for the selected transitions of c-C_9H_8 observed towards TMC-1. The red line shows the computed synthetic spectrum for indene assuming $T_r = 10$ K and $N(c\text{-}C_9H_8) = 1.6 \times 10^{13}$ cm^{-2}. Cyan labels, when present, indicate the multiplicative factor applied to the best fit model to match the observations.

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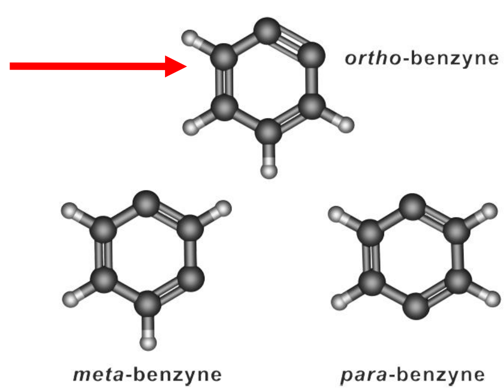
A&A 652, L9 (2021)
https://doi.org/10.1051/0004-6361/202141660

Astronomy & Astrophysics

Letter to the Editor

Discovery of benzyne, o-C_6H_4, in TMC-1 with the QUIJOTE line survey★

J. Cernicharo[1], M. Agúndez[1], R. I. Kaiser[2], C. Cabezas[1], B. Tercero[3,4], N. Marcelino[1], J. R. Pardo[1], and P. de Vicente[3]



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A&A 655, L1 (2021)
https://doi.org/10.1051/0004-6361/202142226

Discovery of two isomers of ethynyl cyclopentadiene in TMC-1: Abundances of CCH and CN derivatives of hydrocarbon cycles★

J. Cernicharo[1], M. Agúndez[1], R. I. Kaiser[2], C. Cabezas[1], B. Tercero[3,4], N. Marcelino[4], J. R. Pardo[1], and P. de Vicente[3]

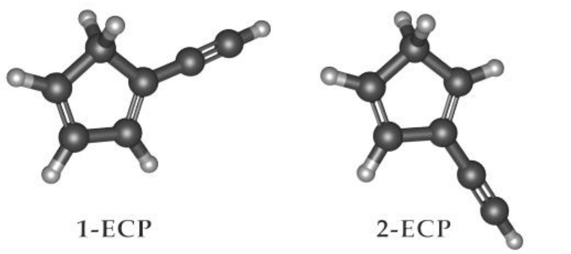

Fig. 1. Scheme of the two lowest energy isomers of ethynyl cyclopen tadiene.

Cyano derivatives of cyclopentadiene detected by GOTHAM team by stacking techniques.

Table 1. Abundances of ethynyl and cyano species in TMC-1.

Molecule	N (cm^{-2})	Abundance[a]	Comments
c-C_5H_6	1.3×10^{13}	1.3×10^{-09}	1
1-c-C_5H_5CCH	1.4×10^{12}	1.4×10^{-10}	2
2-c-C_5H_5CCH	2.0×10^{12}	2.0×10^{-10}	2
1-c-C_5H_5CN	3.1×10^{11}	3.1×10^{-11}	2,A
2-c-C_5H_5CN	1.3×10^{11}	1.3×10^{-11}	2,B
C_6H_5CCH	$\sim2.5\times10^{12}$	2.5×10^{-10}	2,C
C_6H_5CN	1.2×10^{12}	1.2×10^{-10}	2,D
c-C_9H_8	1.6×10^{13}	1.6×10^{-09}	1,E

Notes.
[a] Assuming a column density of molecular hydrogen of 10^{22} cm^{-2} (Cernicharo & Guélin 1987). [1] Cernicharo et al. (2021c). [2] This work. [A] A value of 1.44×10^{12} cm^{-2}, has been reported by McCarthy et al. (2021) and of 8.3×10^{11} cm^{-2} by Lee et al. (2021). [B] A value of 1.9×10^{11} cm^{-2} has been derived by Lee et al. (2021). [C] Tentative detection. [D] A value of 4.0×10^{11} cm^{-2} has been derived by McGuire et al. (2018). This value has been revised to 1.6×10^{11} cm^{-2} by Burkhardt et al. (2021b). [E] A value of 9.6×10^{12} cm^{-2} has been reported by Burkhardt et al. (2021b).

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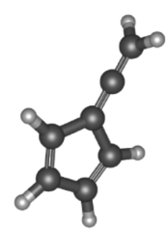
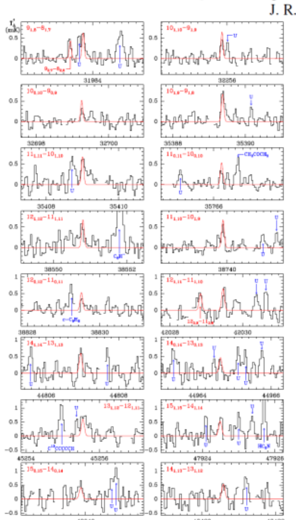
A&A 663, L9 (2022)
https://doi.org/10.1051/0004-6361/202244399

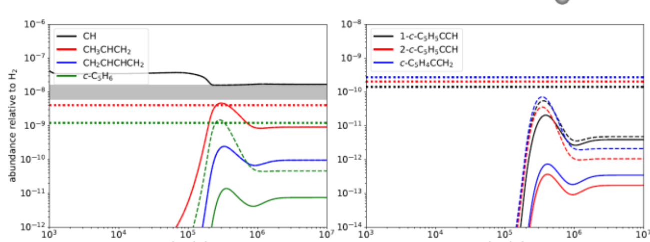
LETTER TO THE EDITOR

Discovery of fulvenallene in TMC-1 with the QUIJOTE line survey★

J. Cernicharo[1], R. Fuentetaja[1], M. Agúndez[1], R. I. Kaiser[2], C. Cabezas[1], N. Marcelino[3,4], B. Tercero[3,4], J. R. Pardo[1], and P. de Vicente[3]







l-$C_3H_3^+$ + C_2H_4 has been measured and it is found to be fast and producing $C_5H_7^+$ (not included in previous models)

Including this reaction, reasonable results on the abundance of cyclopentadiene, and of the hydrocarbons found with QUIJOTE, are obtained

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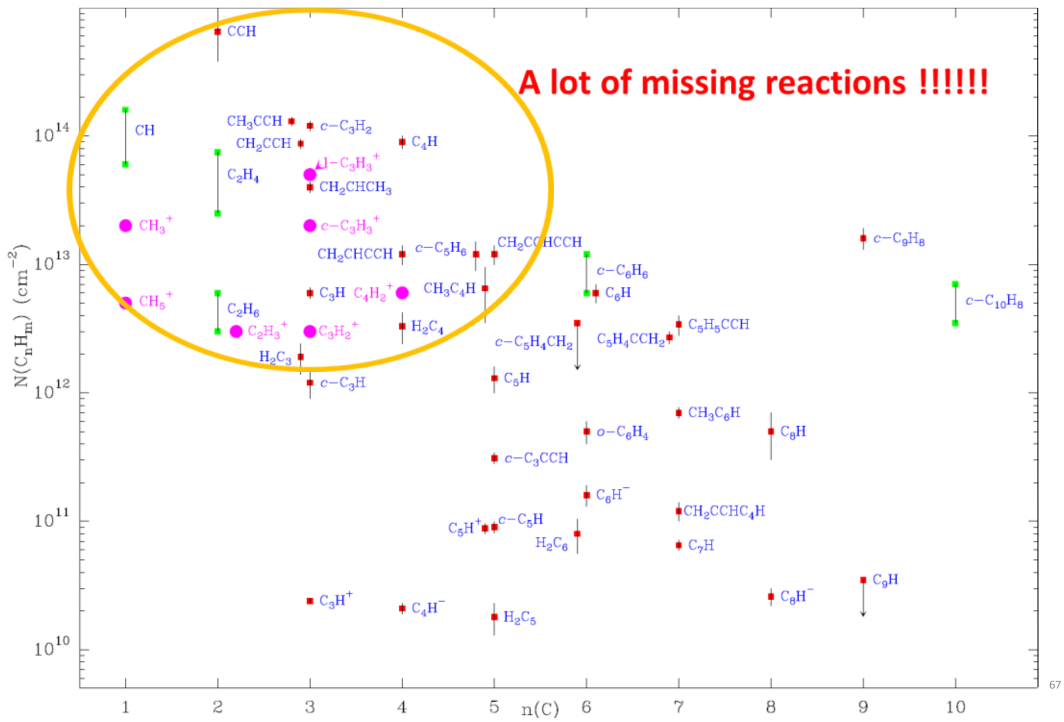

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Summary of QUIJOTE's results in the last four years

- First data (50 hours) arrived in July 2020. By May 2021 the total on-source time was 238 hours; 420 hours by Jan 2022; 540 hours by May 2022; 850 by Feb 2023; 1208 hours Jan 2024
- Since September 2020 we have reported the detection of ~50 new molecular species in TMC-1:
- Ten cations (HC_5NH^+, HC_3S^+, HC_3O^+, CH_3CO^+, C_5H^+, $HCCS^+$, HC_7NH^+, NC_4NH^+, $HCCNCH^+$, $C_3H_3^+$
- One anion (C_7N^-) and confirmation of C_5N^- ($C_{10}H^-$ discovered by GOTHAM; Remijan + 2023)
- Nine neutral sulfur-bearing species (NCS, HCCS, H_2CCS, H_2C_3S, C_4S, HCSCN, HCSCCH, HCCCCS, HSO)
- Eight pure hydrocarbons (CH_2CHCCH, $H_2CCHCCH$, CH_3CH_2CCH, HCCCHCCC, C_3H_3, H_2C_5, CH_2CCHC_4H, c-C_5H)
- Nine new cycles (including indene, cyclopentadiene, ortho-benzyne, two isomers of ethylyn cyclopentadiene, ethynyl cyclopropenylidiene, fulvanallene, ethylynbenzene)
- Three O-rich neutral species (CH_3CHCO, HCCCO, C_5O)
- Eight cyanides and isocyanides (closed shell: HCCCCNC, five isomers of cyano-propene, and open shell species: H_2CCCN, H_2CCCCN, …)
- Still >2500 unidentified lines (below 1mK at 4 σ level)!!!!

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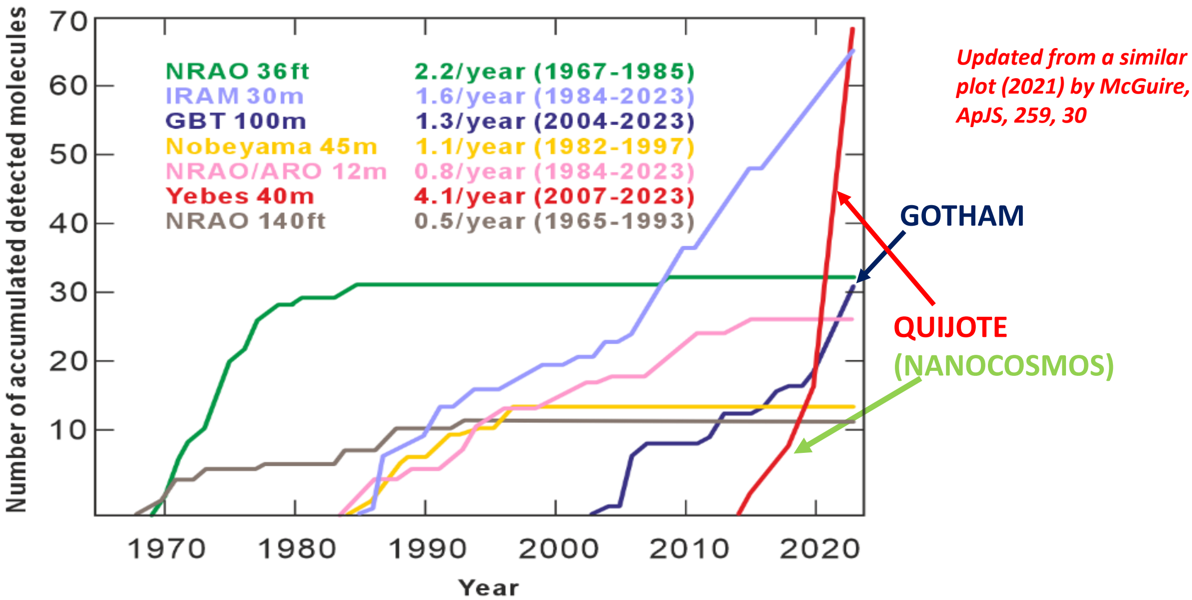

The Yebes 40m telescope (Spain) is the instrument with the largest number of molecular discoveries in space !!!!

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Line surveys are powerful methods to reveal the molecular complexity of a molecular cloud. However…

- Determination of the column density and abundance of a molecule requires to know the spatial size of its emission in each of its lines.
- A single position line survey does not provided enough information to derive spatial information.
- QUIJOTE and GOTHAM beams change by a factor of two within their frequency ranges.
  - QUIJOTE assumes a source size.
  - GOTHAM fits four velocity components with a size for each of them extracting information from stacking. In most cases individual lines are not detected.
  - SANCHO: Surveying the Area of the Neighbour TMC-1 Cloud through Heterodyne Observations

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SANCHO complement to the QUIJOTE line survey
Fully sampled maps covering a region of 240”x240”
2-4 mK/pixel for Yebes 40m telescope and 10-15 mK for the IRAM 30m telescope

A&A 674, L4 (2023)
https://doi.org/10.1051/0004-6361/202346722

Astronomy & Astrophysics

Letter to the Editor

The spatial distribution of an aromatic molecule, C_6H_5CN, in the cold dark cloud TMC-1★

J. Cernicharo[1], B. Tercero[2,3], N. Marcelino[2,3], M. Agúndez[1], and P. de Vicente[2]

ABSTRACT

We present a highly sensitive 2D line survey of TMC-1 obtained with the Yebes 40 m radio telescope in the Q-band (31.13–49.53 GHz). These maps cover a region of 320″×320″ centred on the position of the QUIJOTE line survey with a spatial sampling of 20″. The region covering 240″×240″, where a longer integration time was used, shows a homogenous sensitivity of 2–4 mK across the band. We present in this work the first determination of the spatial extent of benzonitrile (C_6H_5CN), which follows that of cyanopolyynes rather well, but differs significantly from that of the radicals C_nH and C_nN. We definitively conclude that aromatic species in TMC-1 are formed from chemical reactions involving smaller species in the densest zones of the cloud.

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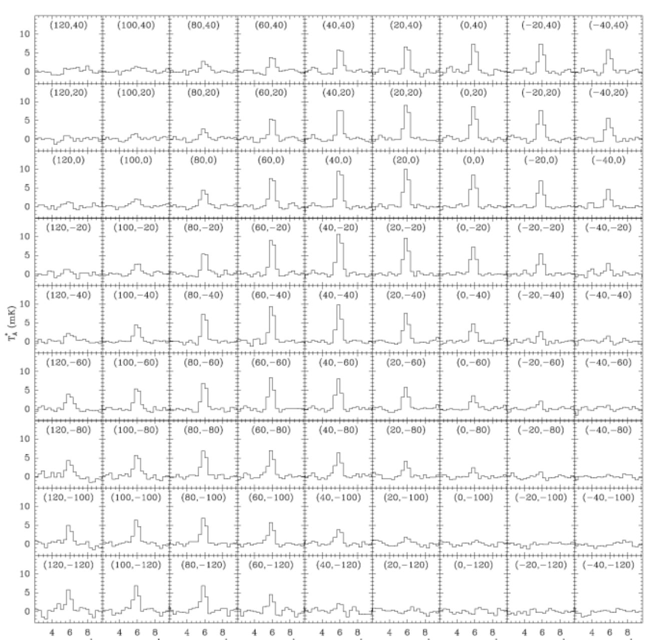
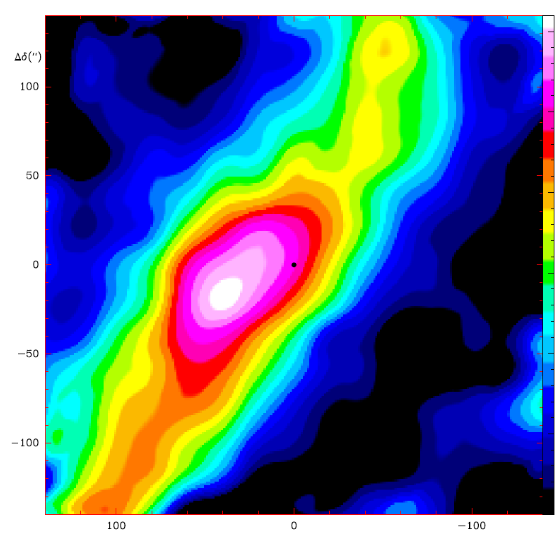


The spatial distribution of benzonitrile in TMC-1



C_6H_5CN as a proxy of C_6H_6 and PAHs in TMC-1.
Bottom-up processes to form PAHs in cold dark clouds

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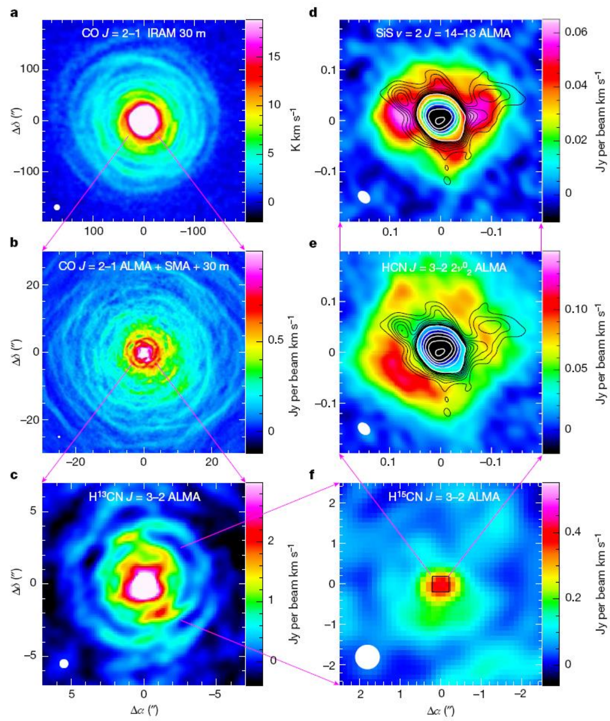

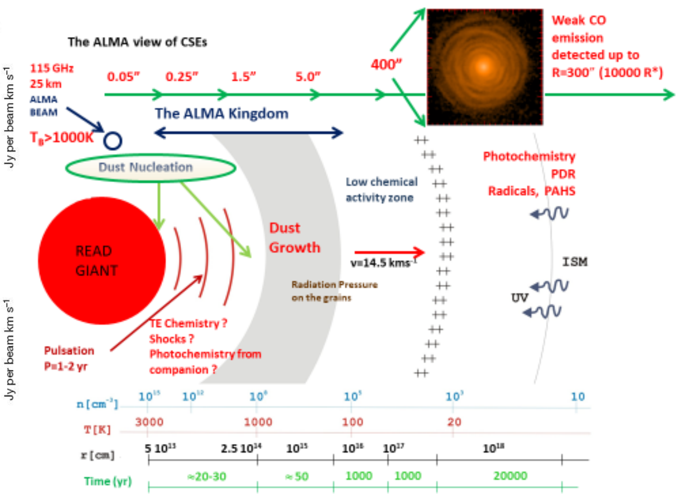

IRC+10216 (CW Leo), Velilla-Prieto et al. 2023, Nature, 617, 696

These C-rich objects were assumed to be the source of PAHs in our galaxy

NONE of the molecules found in TMC-1 are in IRC+10216

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Line surveys of a carbon-rich star (IRC+10216; prototype of C-rich AGB star; assumed to be the objects where PAHs could be formed).

Around 30% of the molecules found in space have been detected towards this source

Polyatomic metal-bearing species are only detected towards the CSE of AGB stars (Mg-bearing)
NaCl, KCl, AlCl, AlF in IRC+10216 (Cernicharo & Guélin 1987, A&A, 183, L10)
NaCN, MgNC, MgCN, AlCN, AlNC, KCN (see Cernicharo et al. 2023 and references therein)
HMgNC, HMgCCCN (Cabezas et al. 2013, A&A, 775, A133, Cabezas et al. 2023, 672, L12)
CaNC, NaCCCN (Cernicharo et al. 2019, A&A, 627, L4; Cabezas et al. 2023, A&A, 672, L12)
MgC_2 (Changala et al. 2022, ApJ, 940, L42)
MgC_3N,MgC_4H (Cernicharo et al. 2019, A&A, 630, L2)
MgC_5N,MgC_6H (Pardo et al. 2021, A&A, 652, L13)
MgC_3N^+, MgC_5N^+,MgC_4H^+, MgC_6H^+ (Cernicharo et al. 2023, A&A, 672, L13)

BUT NONE OF THE HYDROCARBONs FOUND IN TMC-1 WITH QUIJOTE or GOTHAM!!!!!

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Special Thanks to the engineers and technicians of the Yebes Observatory for building the receivers and spectrometers for the NANOCOSMOS project of the European Research Council
Felix Tercero
leader of the optics and frontends group
Juan Daniel Gallego
leader of the HEMT amplifiers group
José Antonio López-Perez, leader of the receivers and spectrometers group
nanoCOSMOS

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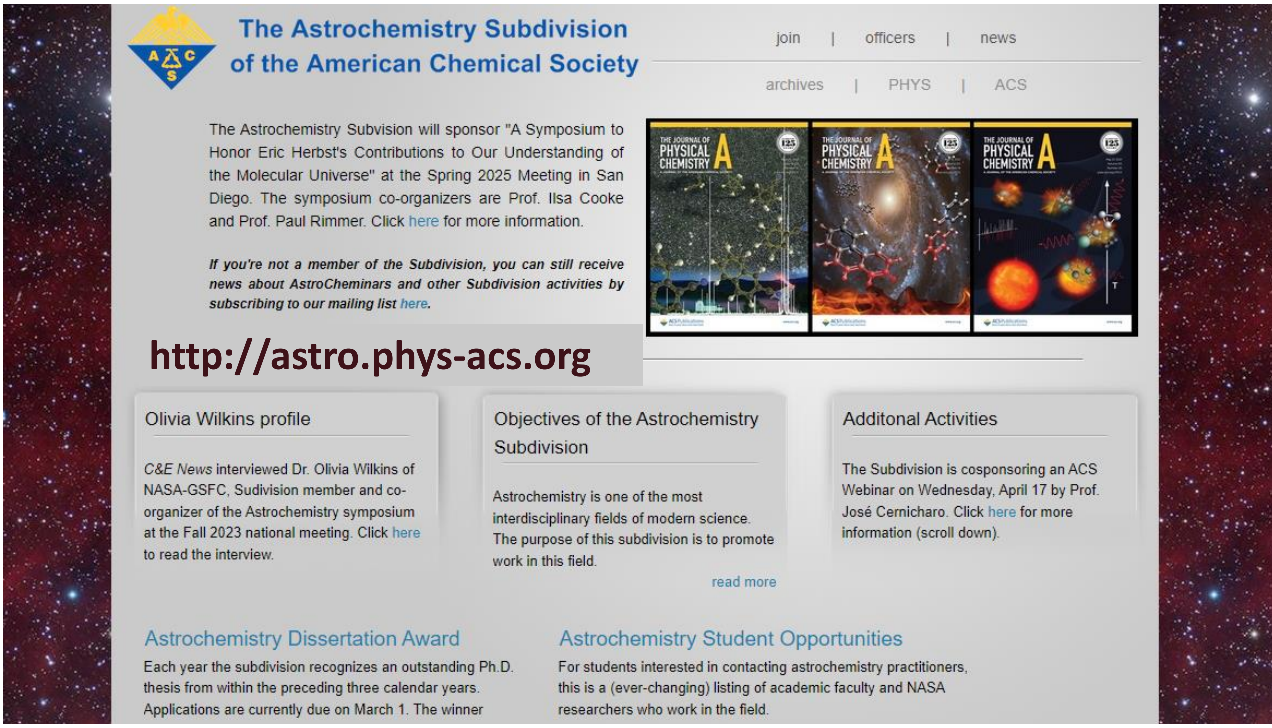

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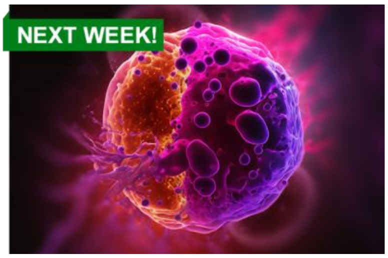

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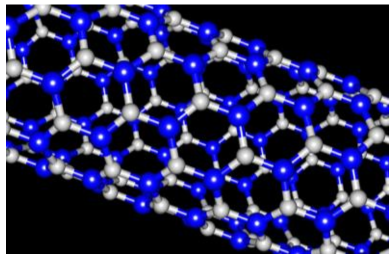

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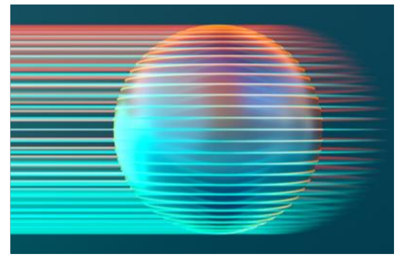

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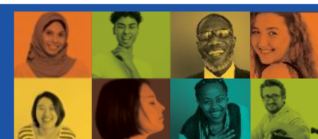

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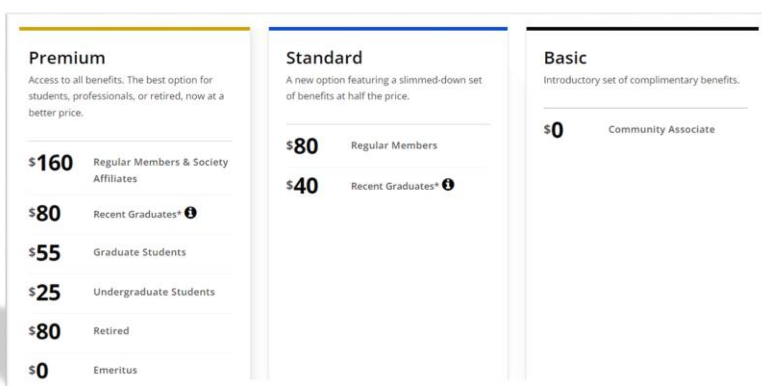

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