



Next
Generation
Astrochemistry



Quest to understand the origin of the Solar system

Nami Sakai (CPR, RIKEN)

Supported by



KAKENHI: Grant-in-Aid for Transformative Research Areas (A) FY2020-FY2024

RIKEN Pioneering Research Project "Evolution of Matter in the Universe (r-EMU)" FY2019-FY2023



Existence of “life” Common or Miracle?



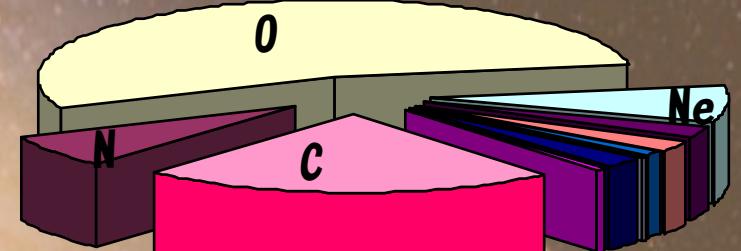
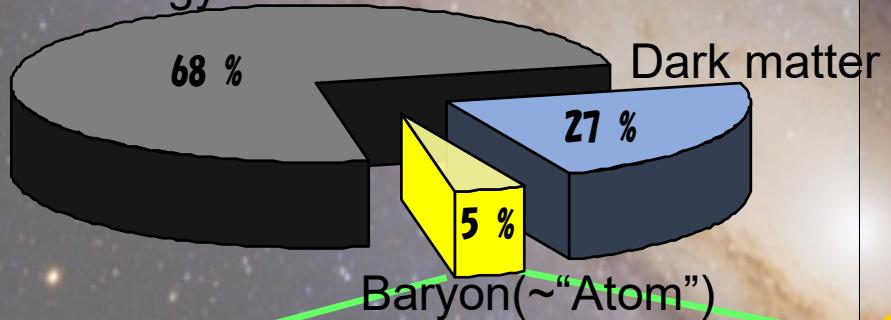
(From NASA)

“Where do we come from?”
→ “How did we get here?”

Why Baryon?

Dark energy

Matter in the Universe

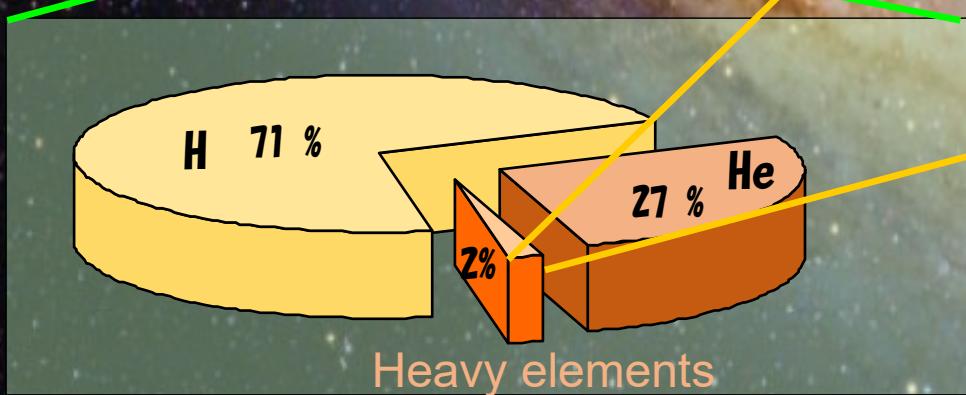


H 71 %

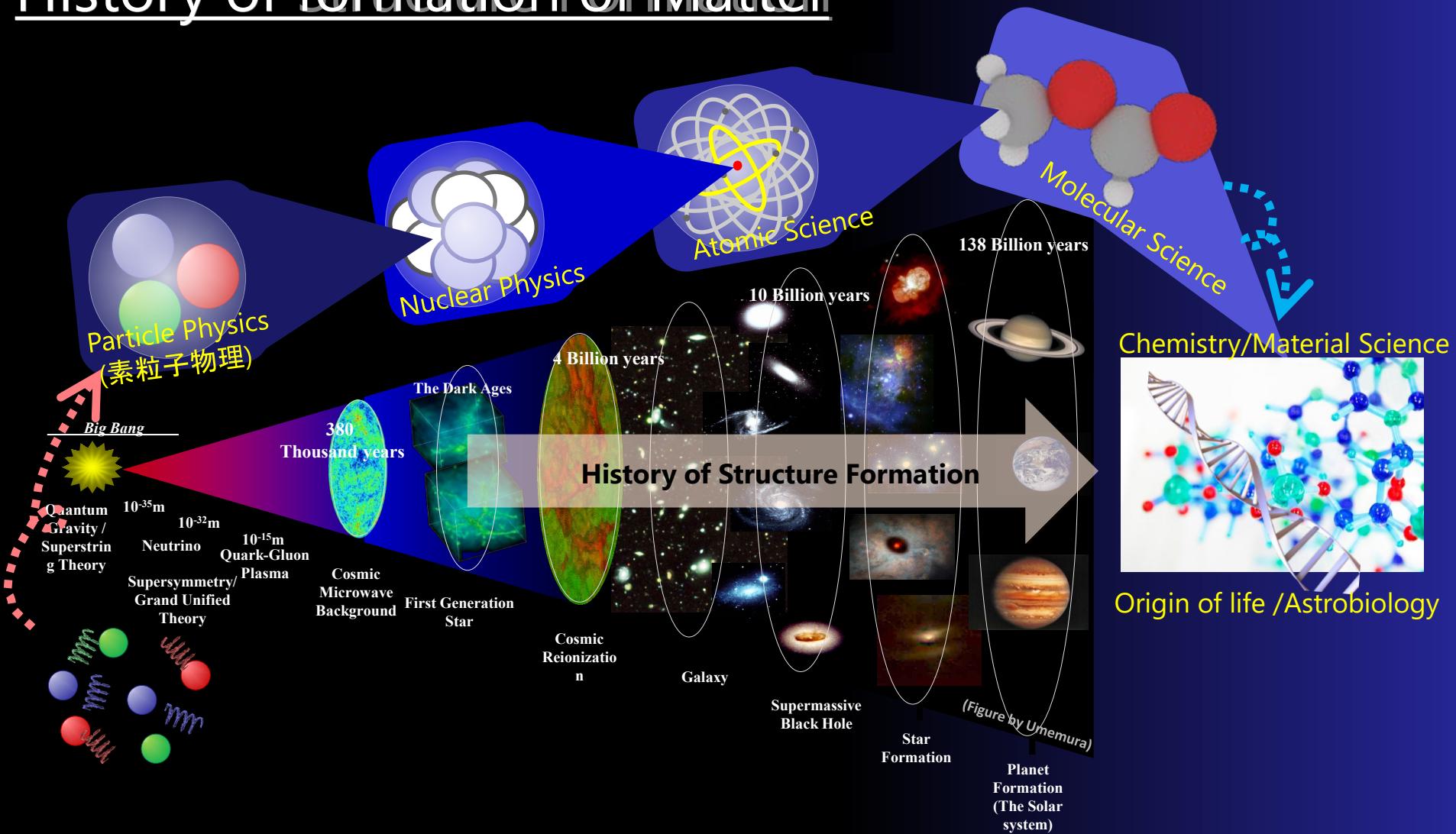
He 27 %

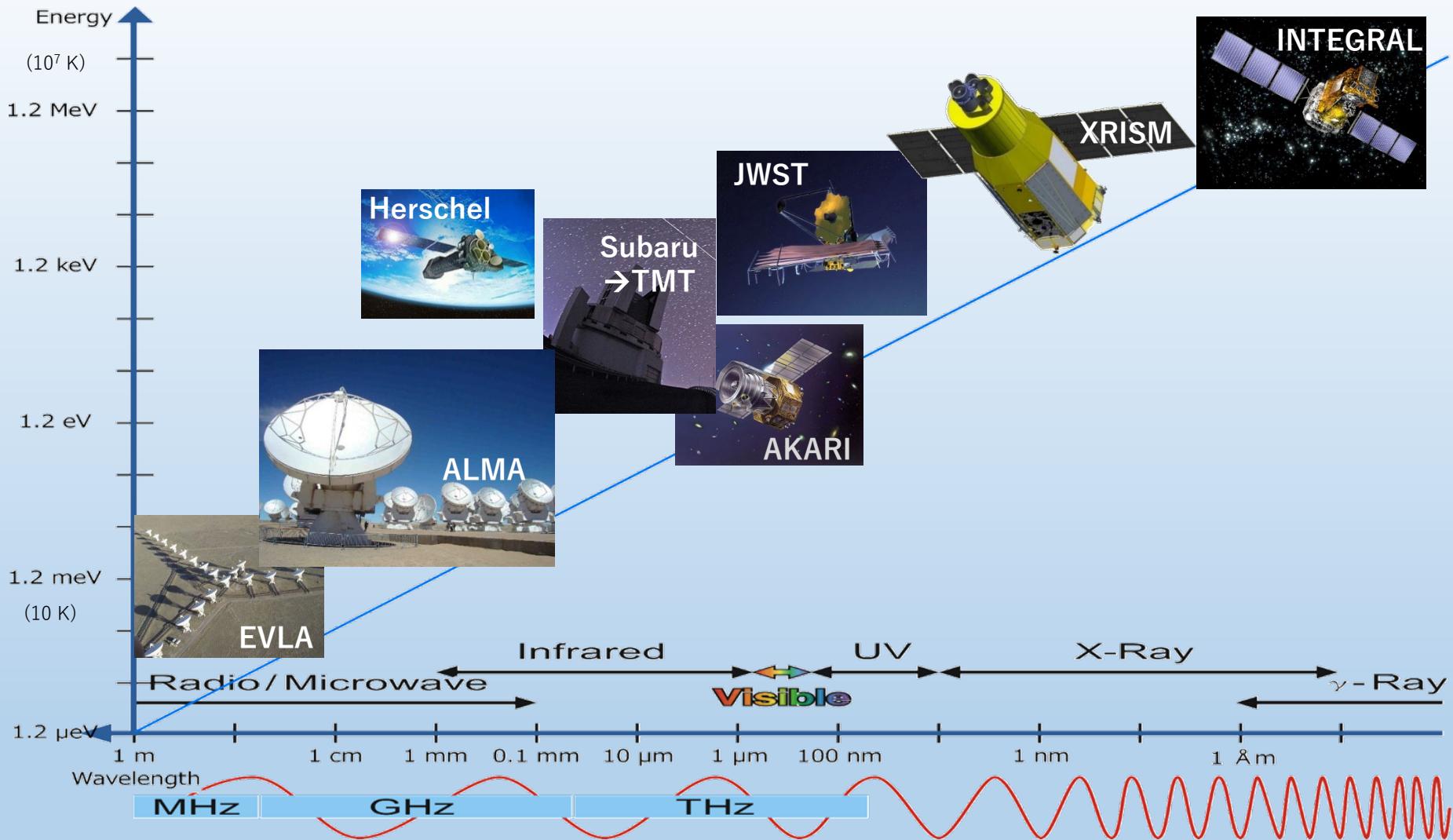
2%

Heavy elements



History of formation of Matter





Molecules in Space (~ 275 species)

2 Atoms (42 Species)

H₂, CO, AlF, AlCl, C₂, CH, CH⁺, CN, CO⁺, CP, SiC, HCl, KCl, NH, NO, NO^{+(?)}, NS, NS⁺, NaCl, OH, PN, SO, SO⁺, SiN, SiO, SiS, CS, HF, HD, FeO (?), O₂, CF⁺, SiH (?), PO, PO⁺, AlO, OH⁺, CN⁻, SH⁺, SH, HCl⁺, TiO, ArH⁺, HeH⁺, NO^{+(?)}, N₂

3 Atoms (40 Species)

C₃, C₂H, C₂O, C₂S, CH₂, HCN, HCO, HCO⁺, HCS⁺, HOC⁺, H₂O, H₂S, HNC, HNO, MgCN, MgNC, N₂H⁺, N₂O, NaCN, OCS, SO₂, c-SiC₂, CO₂, NH₂, H₃⁺, SiCN, AlNC, SiNC, HCP, CCP, AlOH, H₂O⁺, H₂Cl⁺, KCN, FeCN, HO₂, TiO₂, C₂N, Si₂C, HS₂, HCS, HSC, HNO, CaNC, NCS

4 Atoms (27 Species)

c-C₃H, I-C₃H, C₃N, C₃O, C₃S, C₂H₂, NH₃, HCCN, HCNH⁺, HNCO, HNCS, HOCO⁺, H₂CO, H₂CN, H₂CS, H₃O⁺, c-SiC₃, CH₃, C₃N⁻, PH₃, HCNO, HOCN, HSCN, H₂O₂, C₃H⁺, HMgNC, HCCO, CNCN, HONO, MgC₂H, HCCS, HNCN, H₂NC, HCCS⁺

5 Atoms (23 Species)

~~C₅, C₄H, C₄Si, I-C₃H₂, c-C₃H₂, H₂CCN, CH₄, HC₃N, HC₂NC, HCOOH, H₂CNH, H₂C₂O, H₂NCN, HNC₃, SiH₄, H₂COH⁺, C₄H⁻, HC(O)CN, HNCNH, CH₃O, NH₄⁺, H₂NCO⁺, NCCNH⁺, CH₃Cl, MgC₃N, NH₂OH, HC₃O⁺, HC₃S⁺, H₂C₂S, C₄S, HC(O)SH, HC(S)CN, HCCCO~~

Highly unsaturated species (Carbon-chain molecules: CCMs)

↓ iCOMs (interstellar "Complex" Organic Molecules)

6 Atoms (17 Species)

~~C₅H, I-C₄H, C₂H₄, CH₃CN, CH₃NC, CH₃OH, CH₃SH, HC₃NH⁺, HC₂CHO, NH₂CHO, C₅N, I-HC₄H, I-HC₄N, c-H₂C₃O, H₂CCCNH, C₅N⁻, HNCHCN, SiH₃CN, C₅S, MgC₄H, CH₃CO⁺, C₃H₃, H₂C₃S, HCCCHS, C₅O, C₅H⁺, HCCNCH⁺~~

7 Atoms (10 Species)

~~C₆H, CH₂CHCN, CH₃C₂H, HC₅N, CH₃CHO, CH₃NH₂, c-C₂H₄O, H₂CCHOH, C₆H⁻, CH₃NCO, HC₅O, HOCH₂CN, HCCCHNH, HC₄NC, c-C₃HCCN, I-C₅H₂, MgC₅N, CH₂C₃N~~

8 Atoms (11 Species)

~~CH₃C₃N, HC(O)OCH₃, CH₃COOH, C₇H, C₆H₂, CH₂OHCHO, I-HC₆H, CH₂CHCHO, CH₂CCHCN, H₂NCH₂CN, CH₃CHNH, CH₃SiH₃, H₂NC(O)NH₂, HCCCH₂CN, HC₅NH⁺, CH₂CHCCH, MgC₆H, C₂H₃NH₂, (CHOH)₂~~

9 Atoms (10 Species)

~~CH₃C₄H, CH₃CH₂CN, (CH₃)₂O, CH₃CH₂OH, HC₇N, C₈H, CH₃C(O)NH₂, C₈H⁻, C₃H₆, CH₃CH₂SH, CH₃CH₂SH, CH₃NHCHO, HC₇O, HCCCHCHCN, H₂CCHC₃N, H₂CCCCHCCH, HOCHCHCHO(?)~~

10 Atoms (5 Species)

~~CH₃C₅N, (CH₃)₂CO, (CH₂OH)₂, CH₃CH₂CHO, CH₃CHCH₂O, CH₃OCH₂OH, c-C₆H₄, H₂CCCHC₃N, C₂H₅NCO, C₂H₅NH₂(?), HC₇NH⁺~~

11 Atoms (4 Species)

~~HC₉N, CH₃C₆H, C₂H₅OCHO, CH₃OC(O)CH₃, CH₃C(O)CH₂OH, c-C₅H₆, HOCH₂CH₂NH₂~~

12 Atoms (4 Species)

~~c-C₆H₆, n-C₃H₇CN, i-C₃H₇CN, C₂H₅OCH₃, 1-c-C₅H₅CN, 2-c-C₅H₅CN, CH₃C₇N(?), n-C₃H₇OH, i-C₃H₇OH~~

>12 Atoms (3 Species)

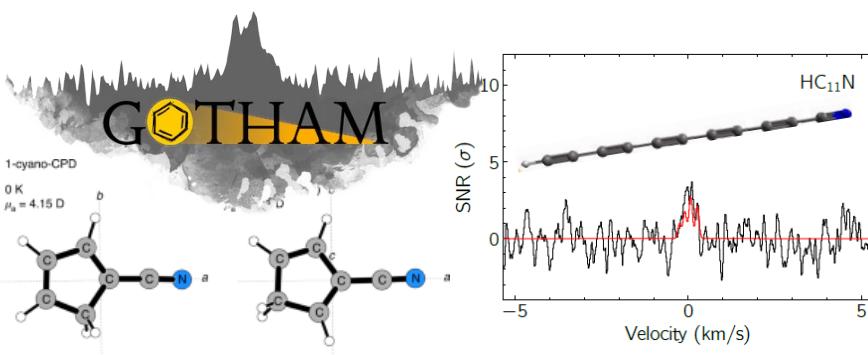
~~C₆₀, C₇₀, C₆₀⁺, c-C₆H₅CN, HC₁₁N, 1-C₁₀H₇CN, 2-C₁₀H₇CN, c-C₉H₈, 1-c-C₅H₅CCH, 2-c-C₅H₅CCH~~

Mainly detected by radio observations

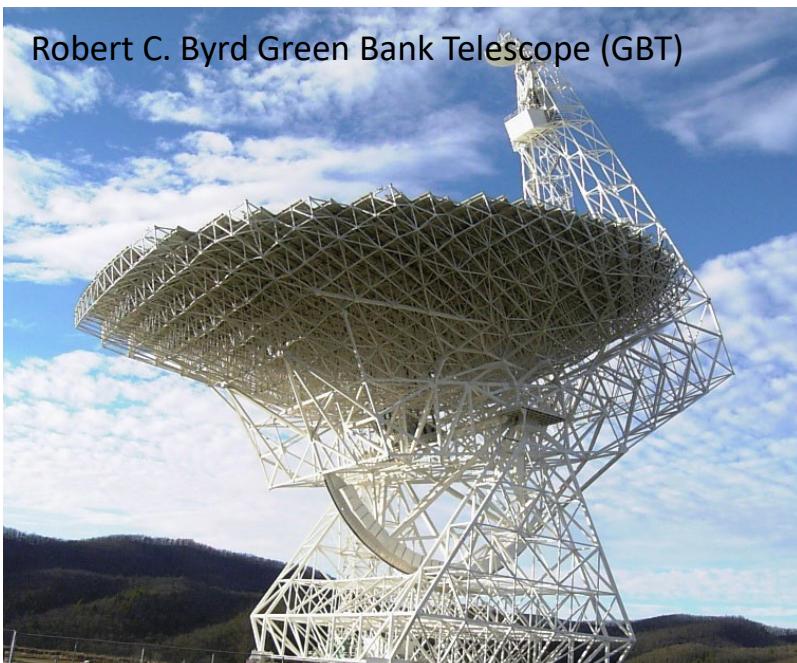
(Gray: Detected only toward AGB stars)

(The Cologne Database for Molecular Spectroscopy (CDMS): June. 2022)

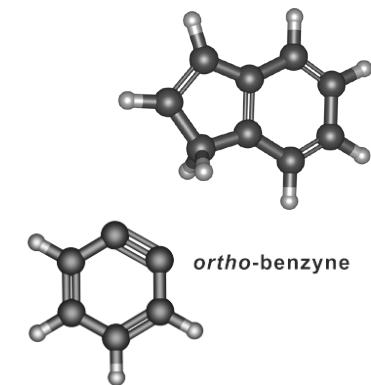
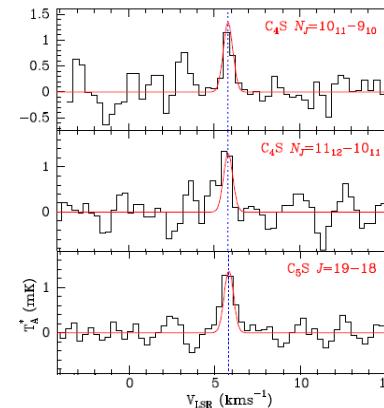
GBT Observations of TMC-1: Hunting Aromatic Molecules (**GOTHAM**)



PI: Brett A. McGuire
(e.g. McGuire, B. A., et al. 2020, ApJ, 900, L10;
McCarthy, M. C., et al. 2021, Natur., 5, 176
Loomis, R. A., et al. 2021, Natur. Astro., 5, 188)



QUIJOTE: Q-band Ultrasensitive Inspection Journey to the Obscure TMC-1 Environment: Discovering the limits of chemical complexity

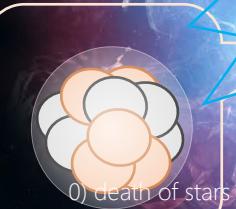
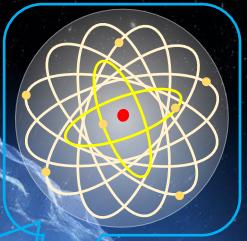


PI: Jose Cernicharo
(Guélin, Michel & Cernicharo, Jose, 2022, Frontiers in Astronomy and Space Sciences, vol. 9, id. 787567, and references therein)

The 40-m Yebes telescope –credit: Pablo deVicente



Formation of atoms
(Nucleosynthesis in stars)
Formation of dust
(M/C Giants, SN)



Nucleus



Evaporation
Gas-phase reactions



Chemical Evolution

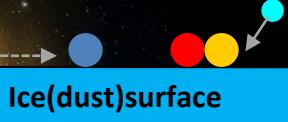
Diffuse Ionized gas $T \sim 100$ K
 → HI cloud (Neutral atoms)
 → Molecular Cloud
 e.g. $O \xrightarrow{H_3^+, H_2} OH \xrightarrow{C} CO$

a) diffuse atomic cloud



$T \sim 10K$
 Density $> 10^5 \text{ cm}^{-3}$
 - Depletion
 - Hydrogenation
 e.g. $CO \rightarrow CH_3OH$

b) molecular cloud (gas and dust)



c) dense cloud core

e) protostar and protoplanetary disk

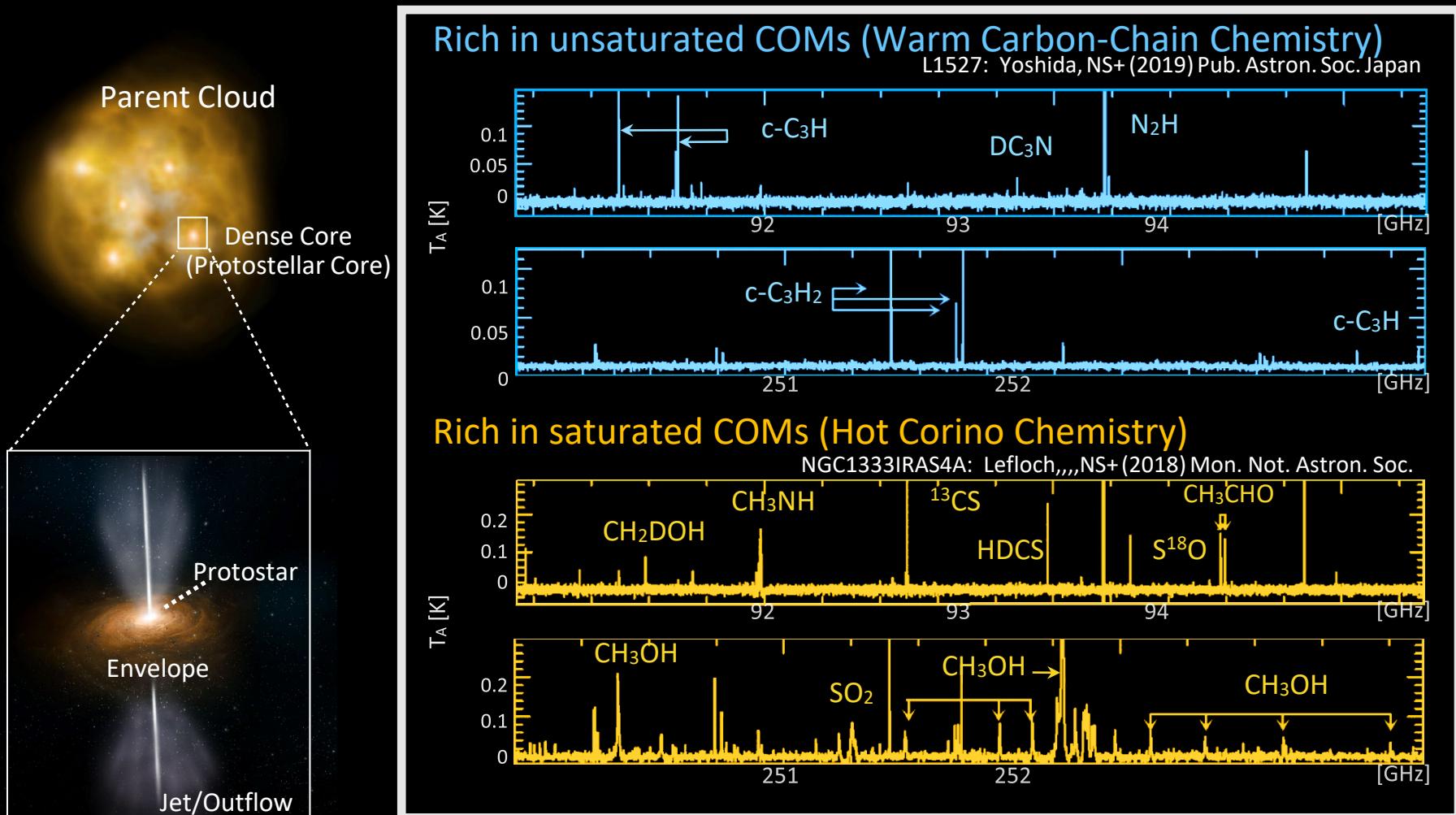


d) protostar, protostellar-envelope/disk, and outflow/jet

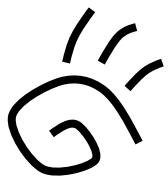
$20K < T < 100K$

Dynamical change of physical condition, Diffusion of heavier elements on dust, Gas-dust interaction → Complex organics

Chemical Composition in Cloud-Core (Envelope) Scale



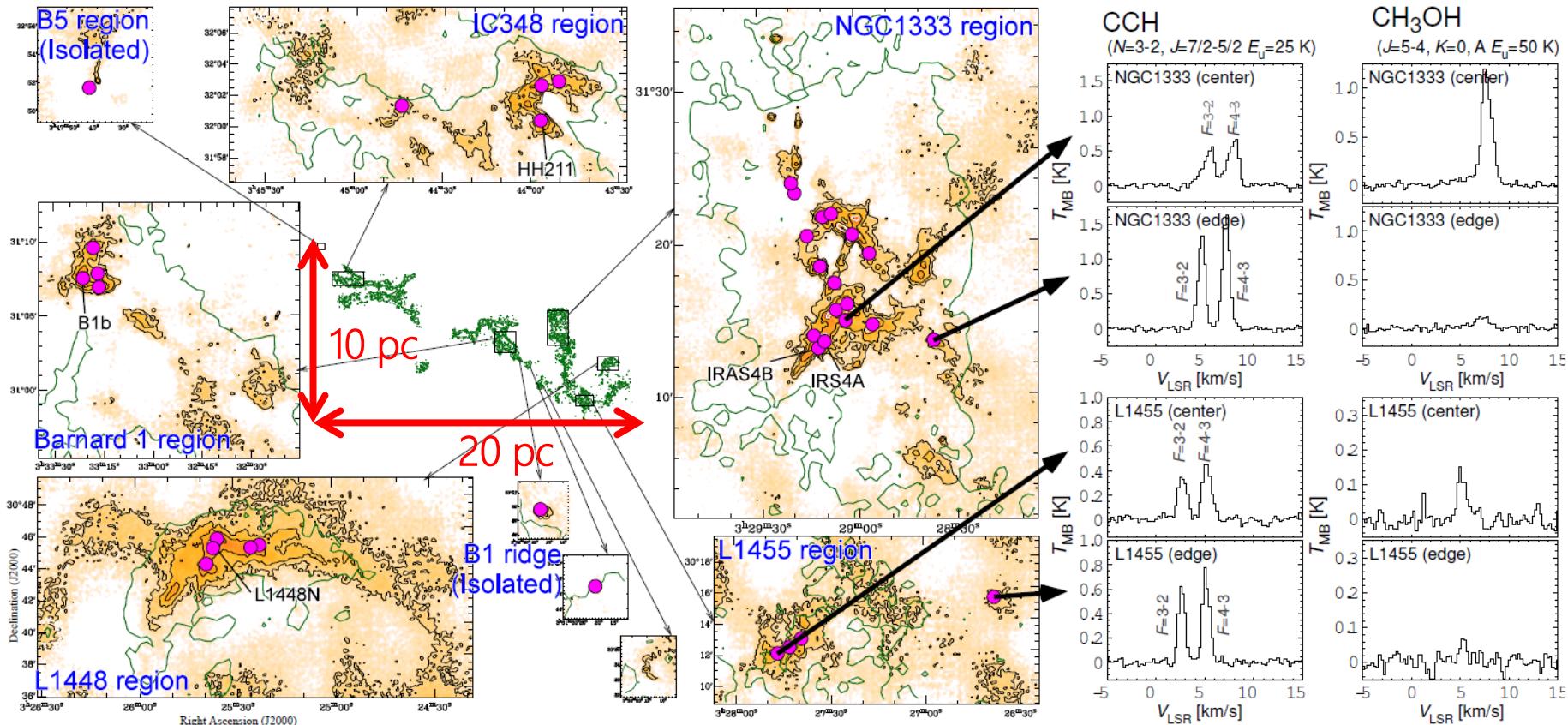
Which is the dominant case ? Which is the case for our solar system??



Perseus Chemical Survey

Exploring core ($\sim 5,000$ au) scale diversity

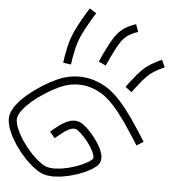
(Nobeyama 45 m + IRAM 30 m survey toward Class0/I sources@2014-2016)



Orange: Dust, Green Contour: CO

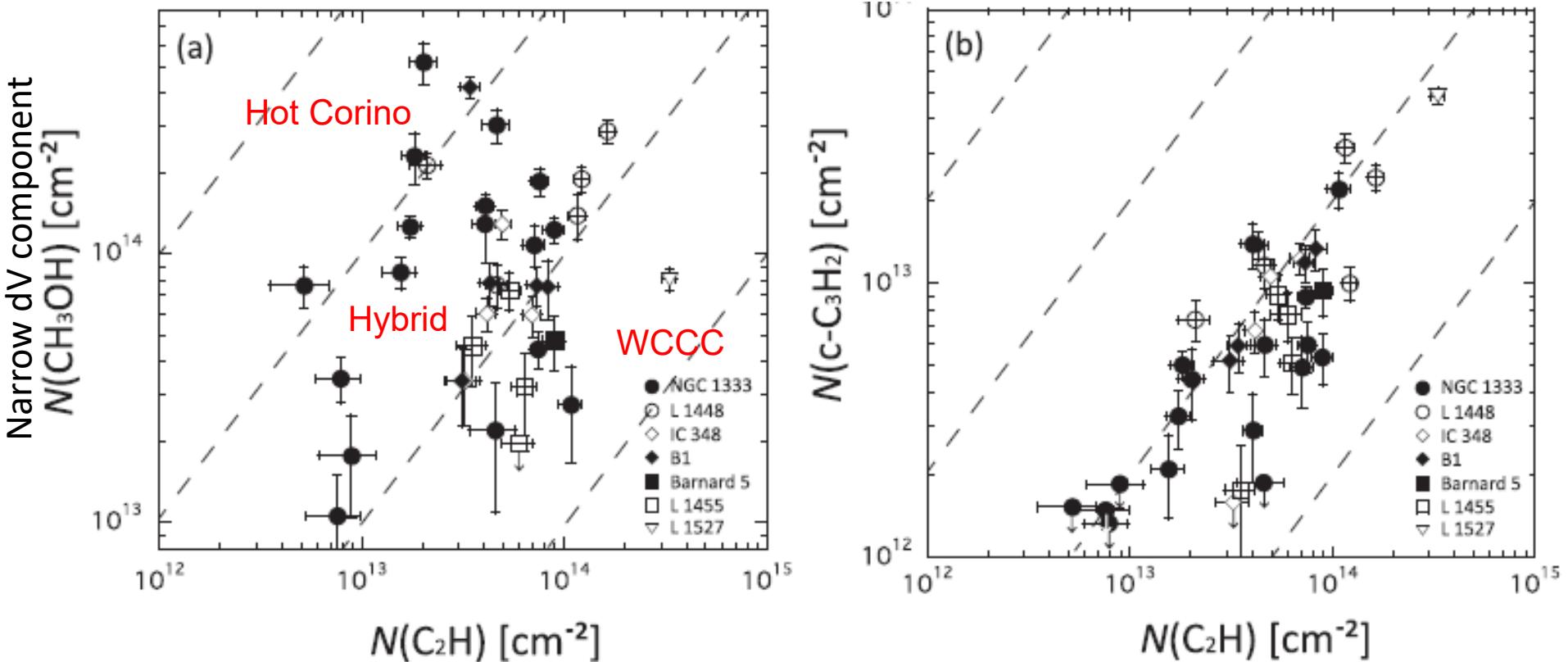
(Hatchell et al. 2005, A&A, 440, 141; 2007, A&A, 468, 1009)

(Higuchi, NS et al. 2018, ApJS, 236, 52)



Chemical Diversity in Perseus

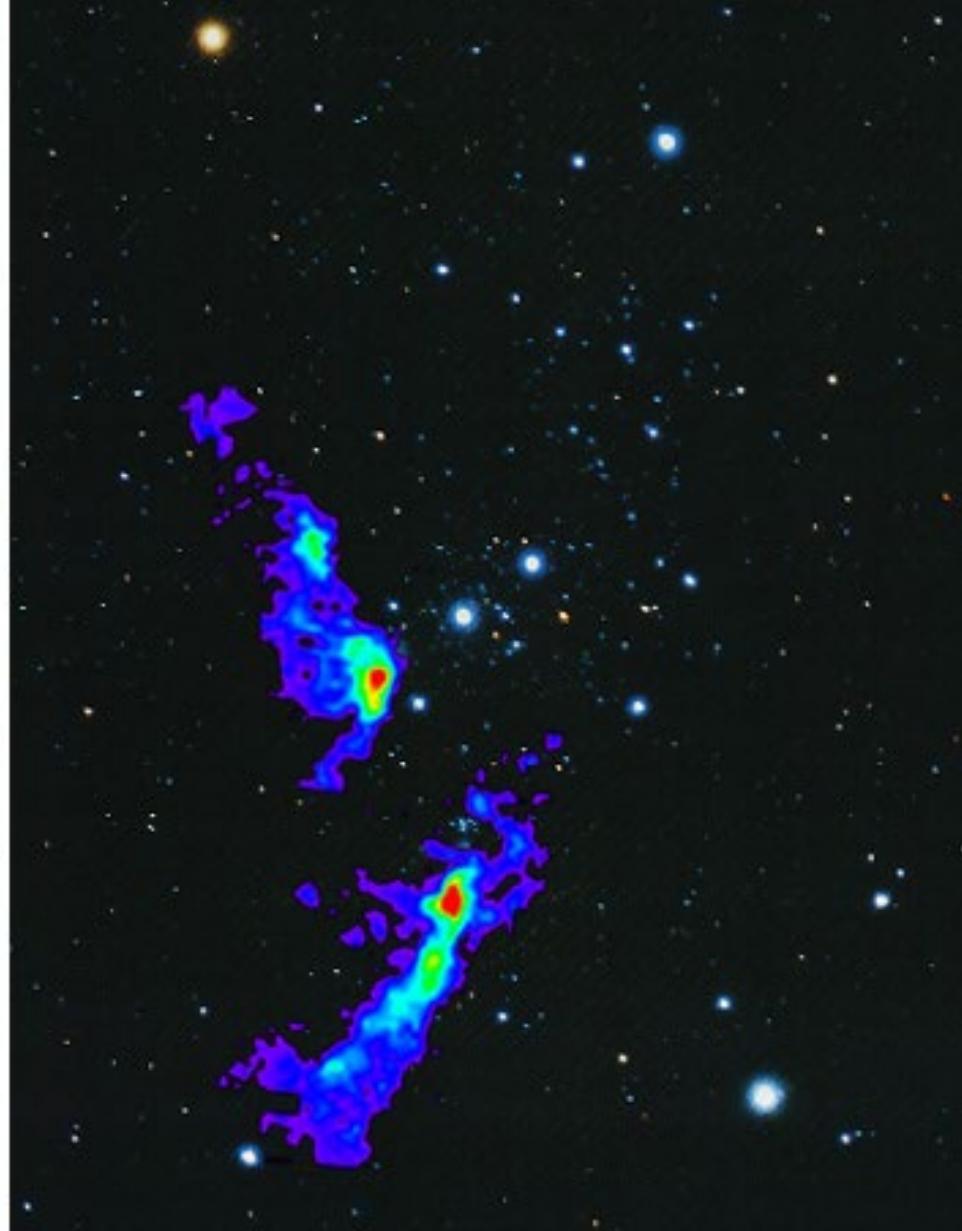
Diversity in envelope size scale ($\sim 5,000$ au)



How about in protoplanetary-disk size scale ?
~100 au

Radio Telescope : Lower Spatial Resolution

Single-Dish: a few 10s arcsec cf; SUBARU (Infrared–Optical) : 0.2–0.02 arcsec



ドイツ: MPIfR 100 m電波望遠鏡





The Robert C. Byrd
Green Bank Telescope,
commonly known as the GBT



ROBERT C. BYRD 300
GREEN BANK TELESCOPE

Scientists take lemons and make lemonade.

The NRAO was able to do more than just replace the 300-foot telescope. In fact, the loss of the big dish became a catalyst for a totally new, unconventional telescope design. The GBT's offset optics and active surface are unique among large radio telescopes. The GBT is the world's largest, fully steerable radio telescope.

United States Senator Robert C. Byrd helped secure congressional funding for the telescope project.

Think you're having a bad day? Sometimes telescopes have them too!

NRAO, Green Bank, West Virginia

9:43 p.m., Tuesday, November 15, 1988

Green Bank's largest telescope collapsed.

Metal fatigue in the antenna's support was determined to be the cause. After delivering 26 years of service (far beyond its life expectancy) the 300-foot diameter telescope dish sank to its foundation, beyond repair.

The loss of the 300-foot telescope resulted in the Green Bank Telescope Project.



BEFORE



AFTER

ALMA: Atacama Large Millimeter/sub-millimeter Array

High angular resolution
 $1'' \rightarrow <0.01''\text{-}0.1''$

High sensitivity
100 hours \rightarrow 10 min.



Main antenna : 12 m x 50

ACA antenna: 12 m x 4, 7 m x 12

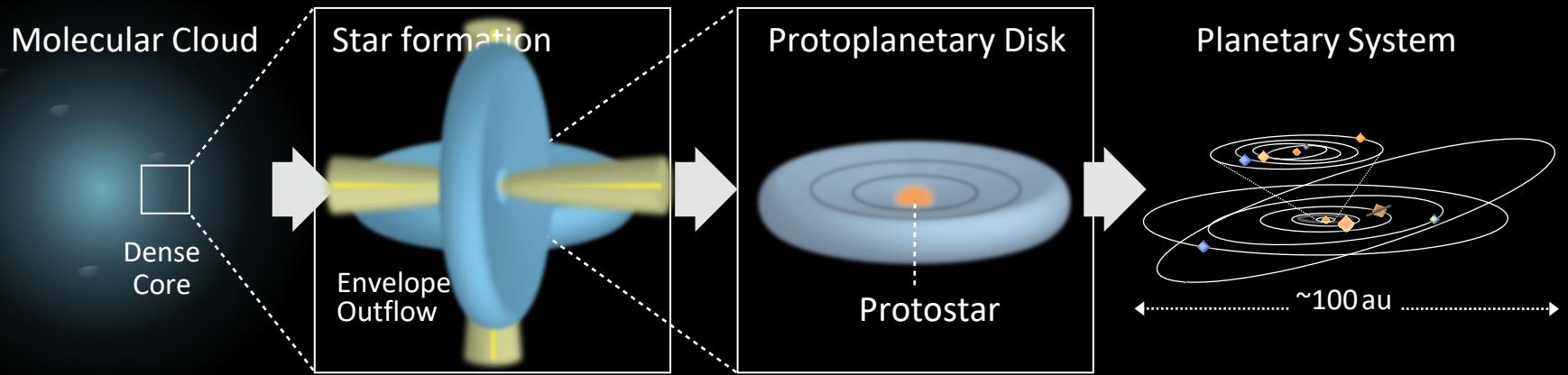
Total:66



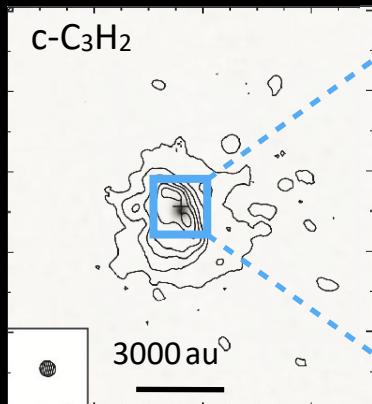
7 mm – 0.4 mm
(40 – 940 GHz)

2014, full operation started
Europe, North America, and East Asia in cooperation with Chile

Formation of Planetary System & Observational Challenges

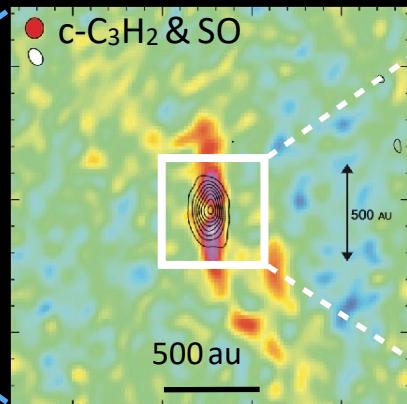


Cloud Core



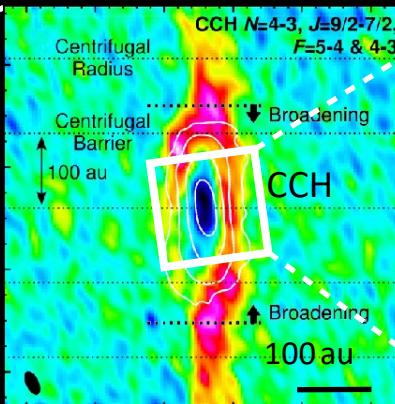
Association/ Infall
Sakai+ (2010)
Astrophys. J.

Envelope



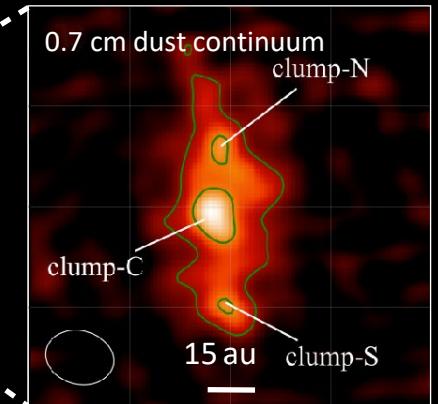
Centrifugal Barrier
Sakai+ (2014)
Nature

Disk



Accretion (soft) shock
Sakai+ (2017)
Mon. Not. R. Astron. Soc.

Disk Substructure
Planet Formation



Nakatani, Sakai+ (2020)
Astrophys. J., 895, L2

Warped : Sakai+ (2019) Nature, 565, 206

PdBI

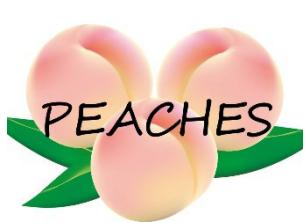


ALMA



VLA





PERseus ALMA CHEmical Survey

Next Generation Astrochemistry

ALMA data:
PI Sakai
~50 YSOs
in Perseus
d~300 pc

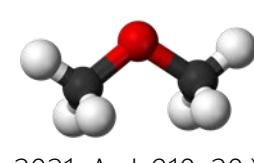
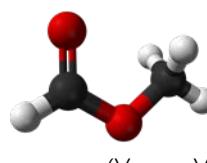
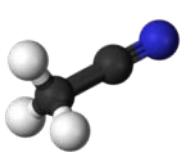
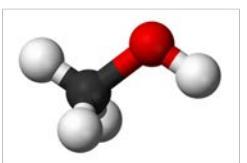
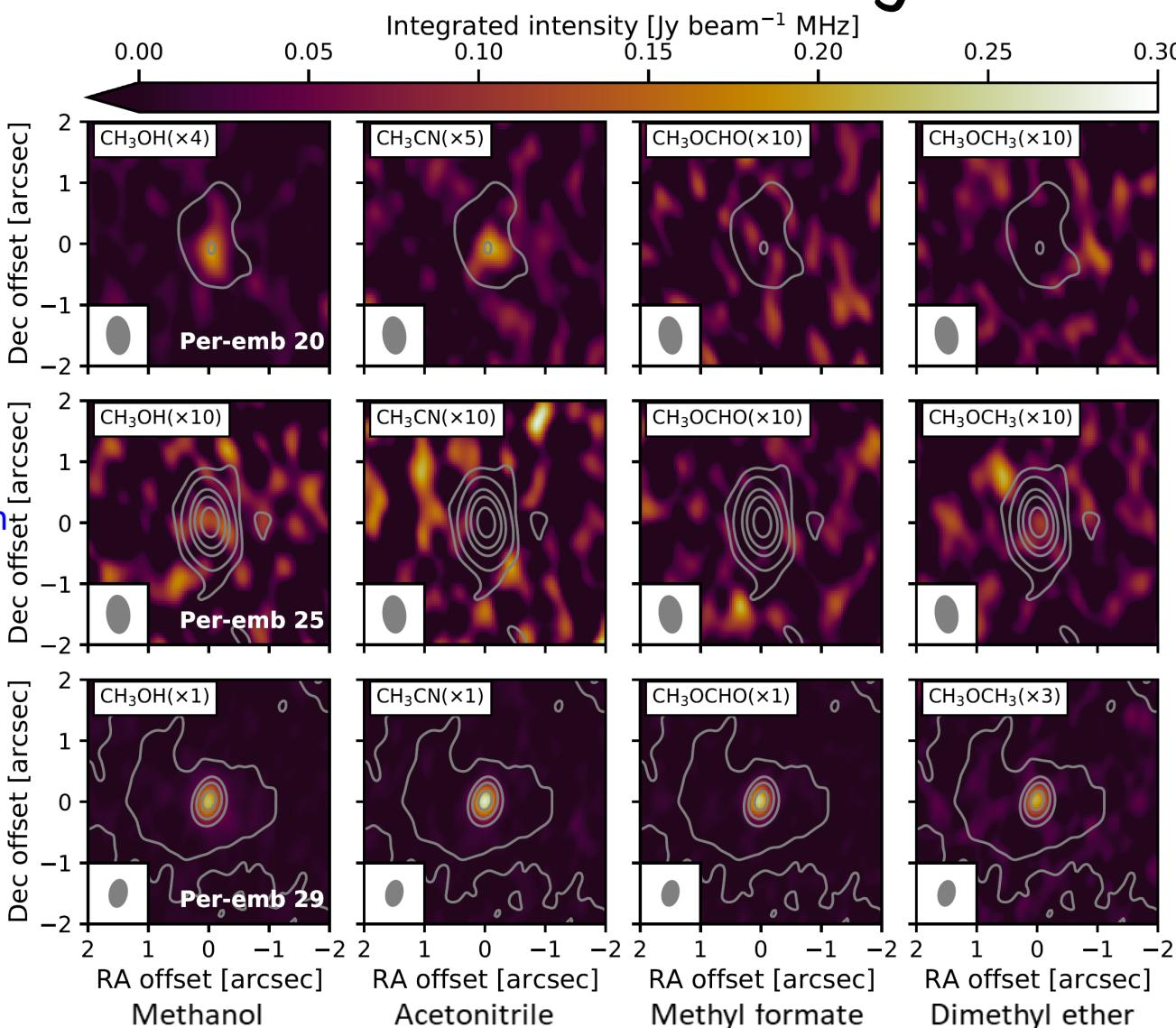
Weakest cont.

Strong cont.
COMs non-detection
(SO/SO₂ detection)

Strongest cont.

Contours: Continuum@1.3mm
0.0006, 0.003, 0.015, 0.03, 0.06 [Jy/beam]

COMs are found in
58% of the sources!



(Yang, Y-L, NS+2021, ApJ, 910, 20.)

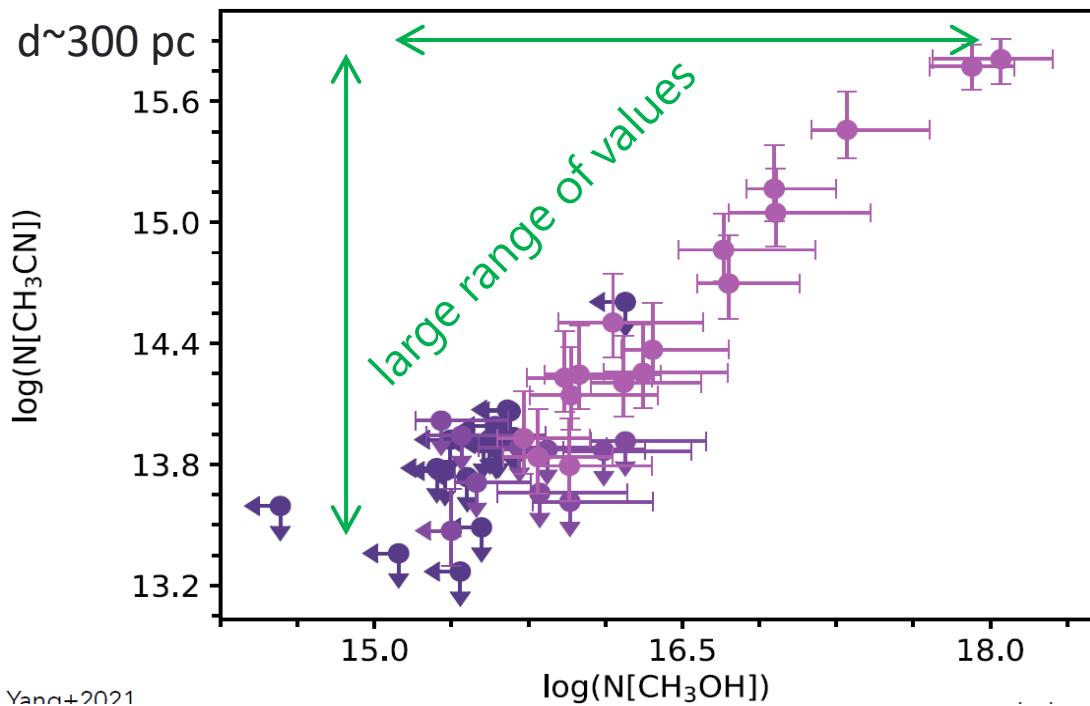


ALMA data:

PI Sakai

~50 YSOs
in Perseus

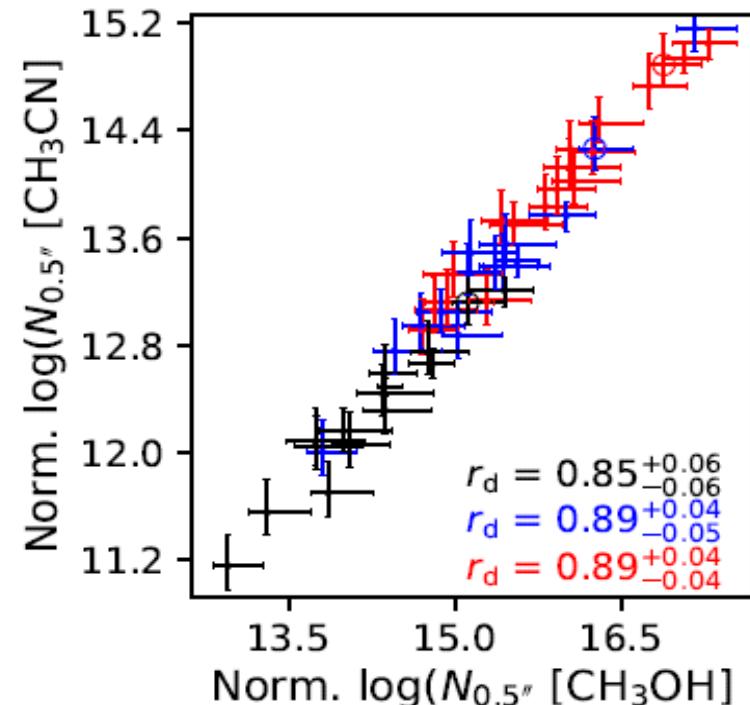
$d \sim 300$ pc



Oxygen vs Nitrogen Chemistry

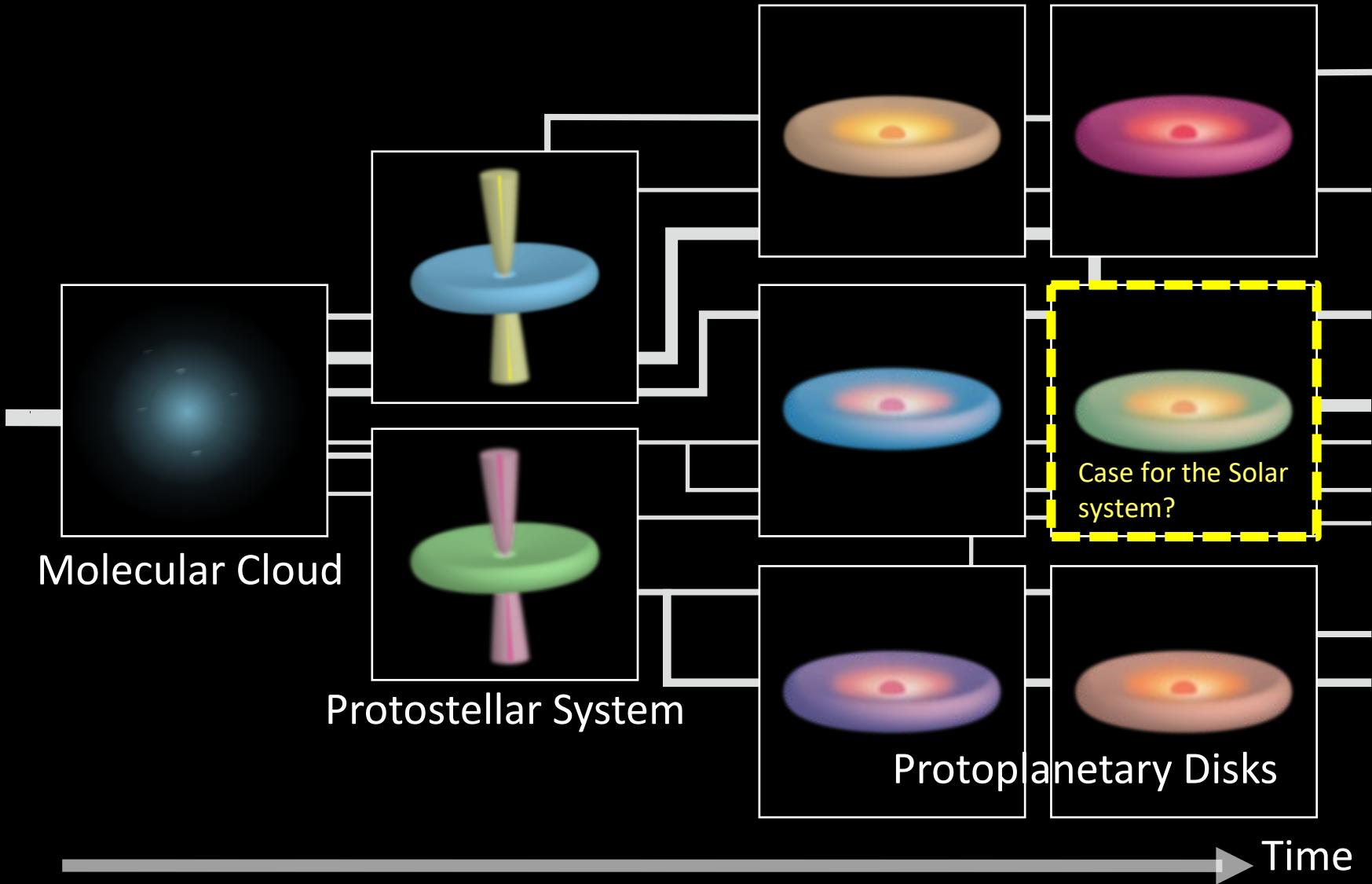
Normalized by

$T_{\text{b,cont}}$, $T_{\text{b,cont}} L_{\text{bol}}$, $T_{\text{b,cont}} T_{\text{bol}}$

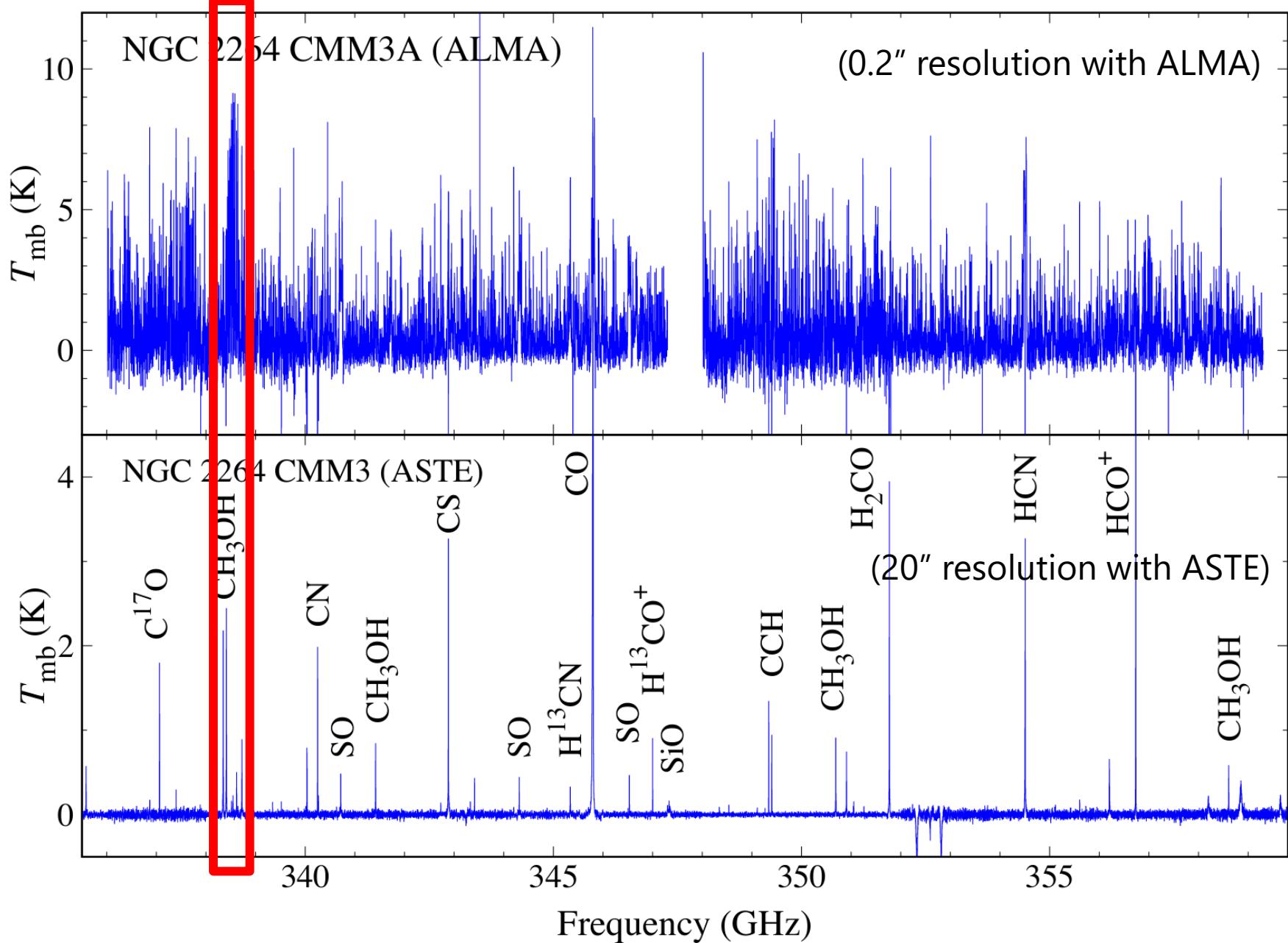


Beautiful correlation between CH_3OH and CH_3CN
 Chem. relation & Large abundance range ($> 10^2$ times).

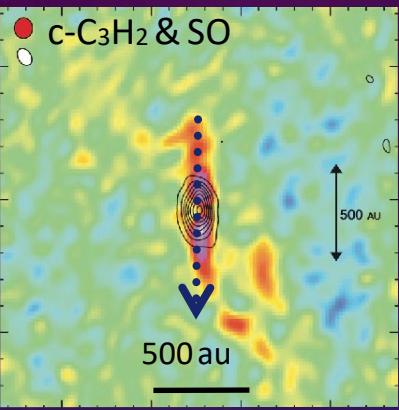
Locate our Solar system in the diversity



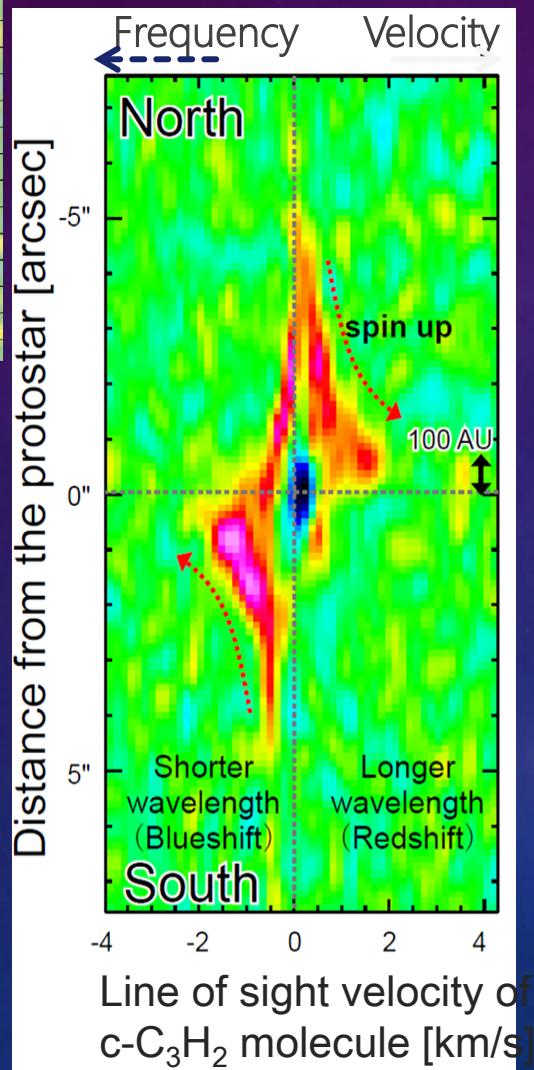
Spectrum taken toward NGC2264CMM3A



Required accuracy for Doppler analysis



Centrifugal Barrier
Sakai+ (2014)
Nature



Thermal line width ~ 0.1 km/s

$\rightarrow \ll 250$ kHz @ 800 GHz = 0.8 THz
(Various high excitation lines)
ALMA

$\rightarrow \ll 50$ kHz @ 160 GHz
(iCOMs)
ALMA/NOEMA & IRAM-30m

$\rightarrow \ll 5$ kHz @ 16 GHz
(Larger iCOMs e.g. with rings)
VLA & GBT/Yabes-40m

Infrared Thermometers

-Measure energy from stars



Check human body for a fever

by measuring the heat energy

→ Ideal for anyone who may have to worry about cross contamination such as infants.



Technology Developed for Astronomy
Meets
Molecular Science ?

Heterodyne Radio-Receiver

-Observe molecules in space

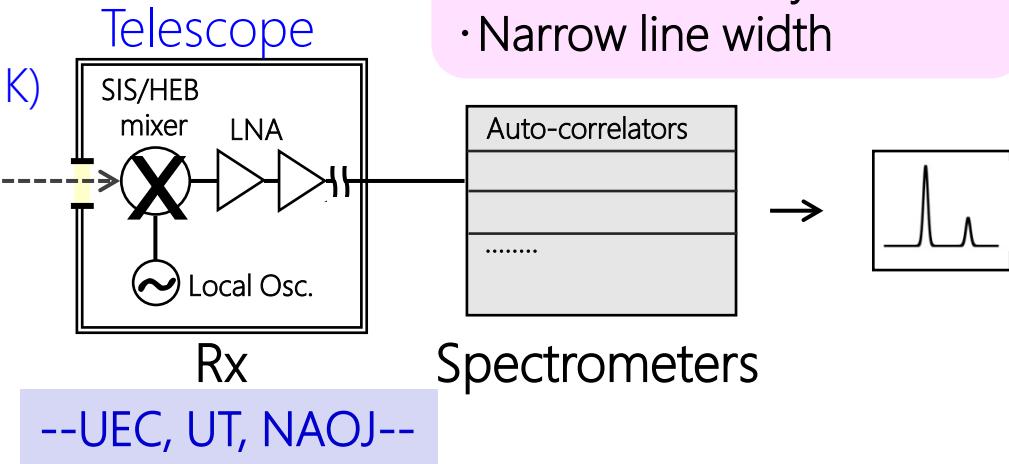
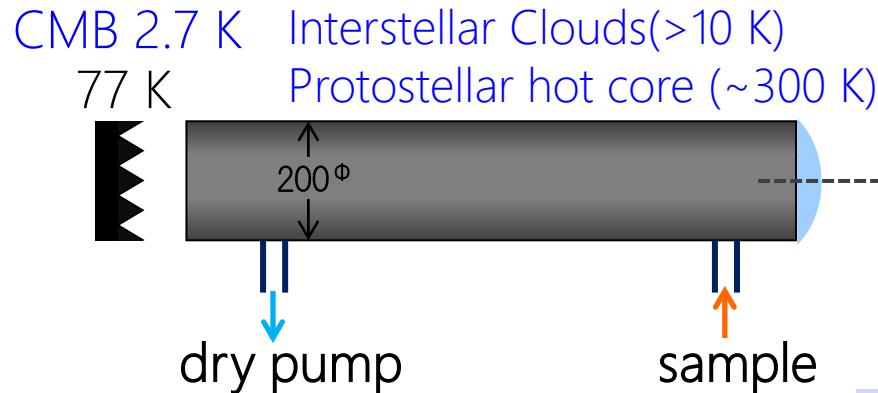


Intensity Measurement of Lines from Molecules

Determine temperature and abundance without direct interaction with the gas.

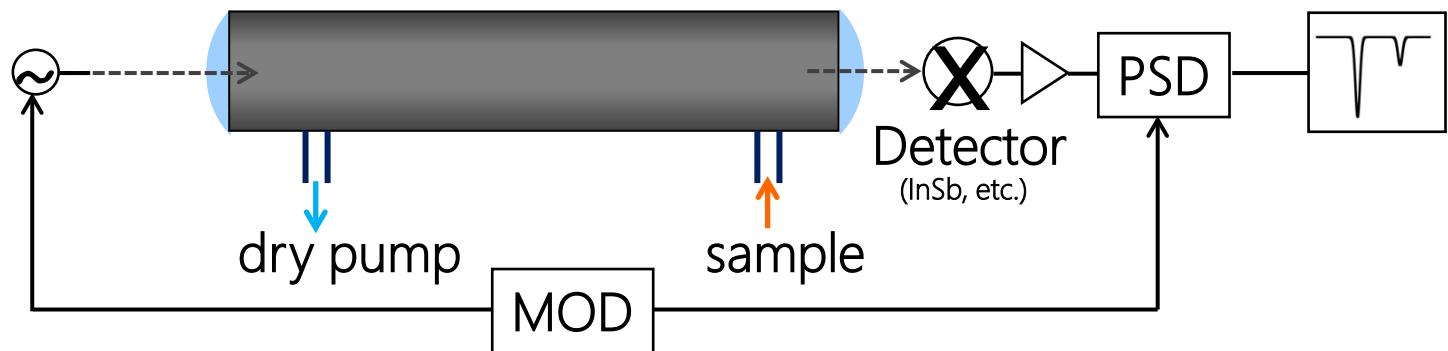
Observing Gas Cell instead of the Sky

Emission Spectrometer



- Wide frequency coverage
- Reliable intensity
- Narrow line width

Conventional Absorption Spectrometer

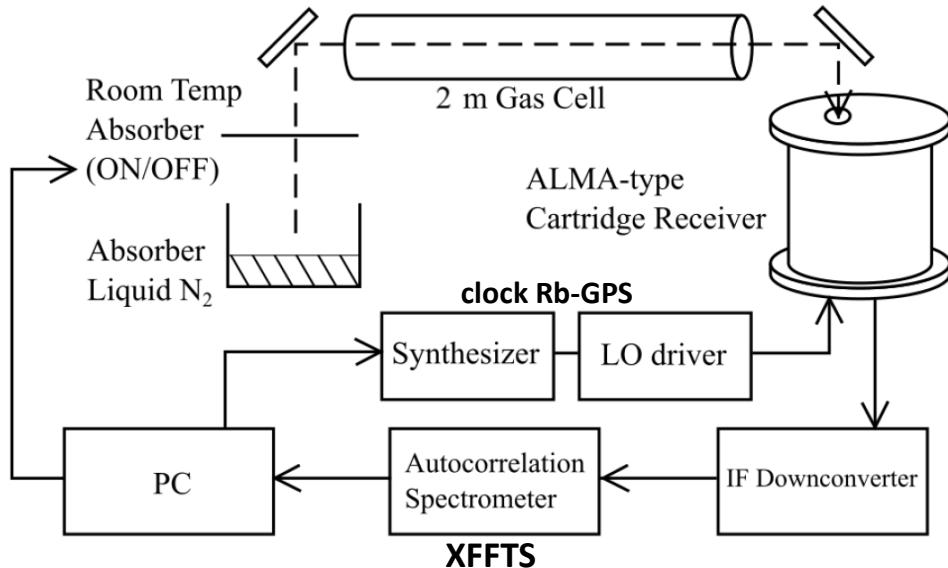
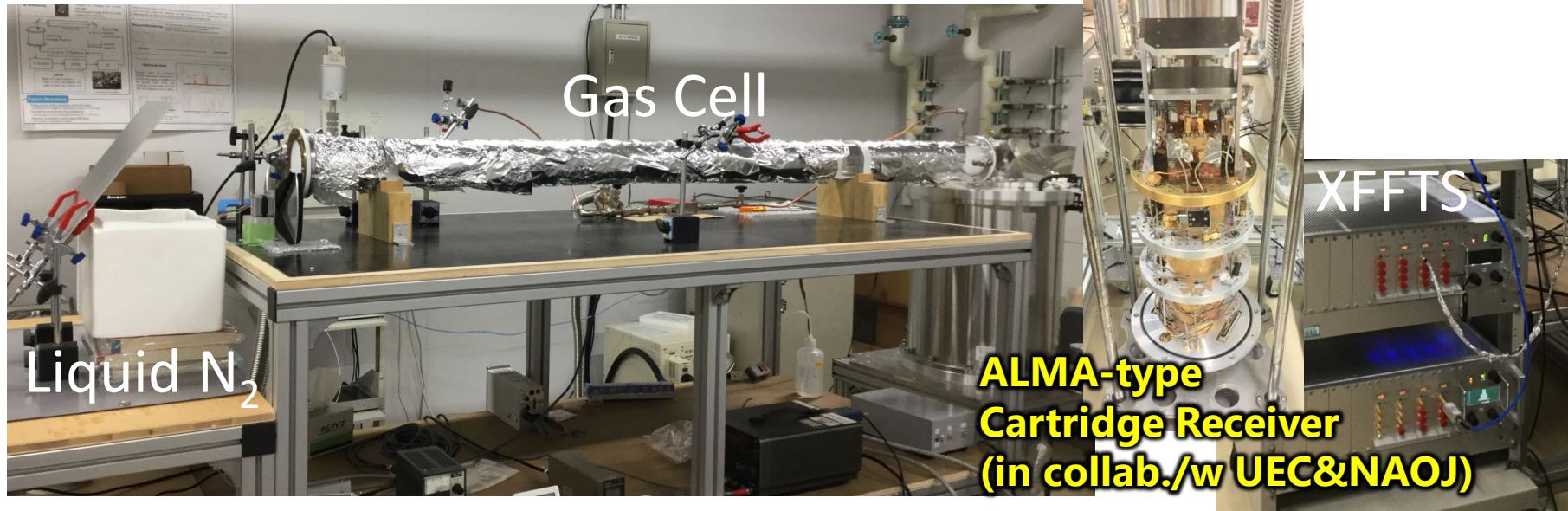


Disadvantage: low sensitivity for 1 line detection



SUMIRE “Observing” gas-cell instead of the sky

Spectrometer Using superconductor MiXer REceiver in RIKEN



Receivers

- 215-265 GHz band (ALMA-B6, SIS)
- 270-500 GHz band (ALMA-B7+8, SIS)

Freq. accuracy: ~ 1 kHz

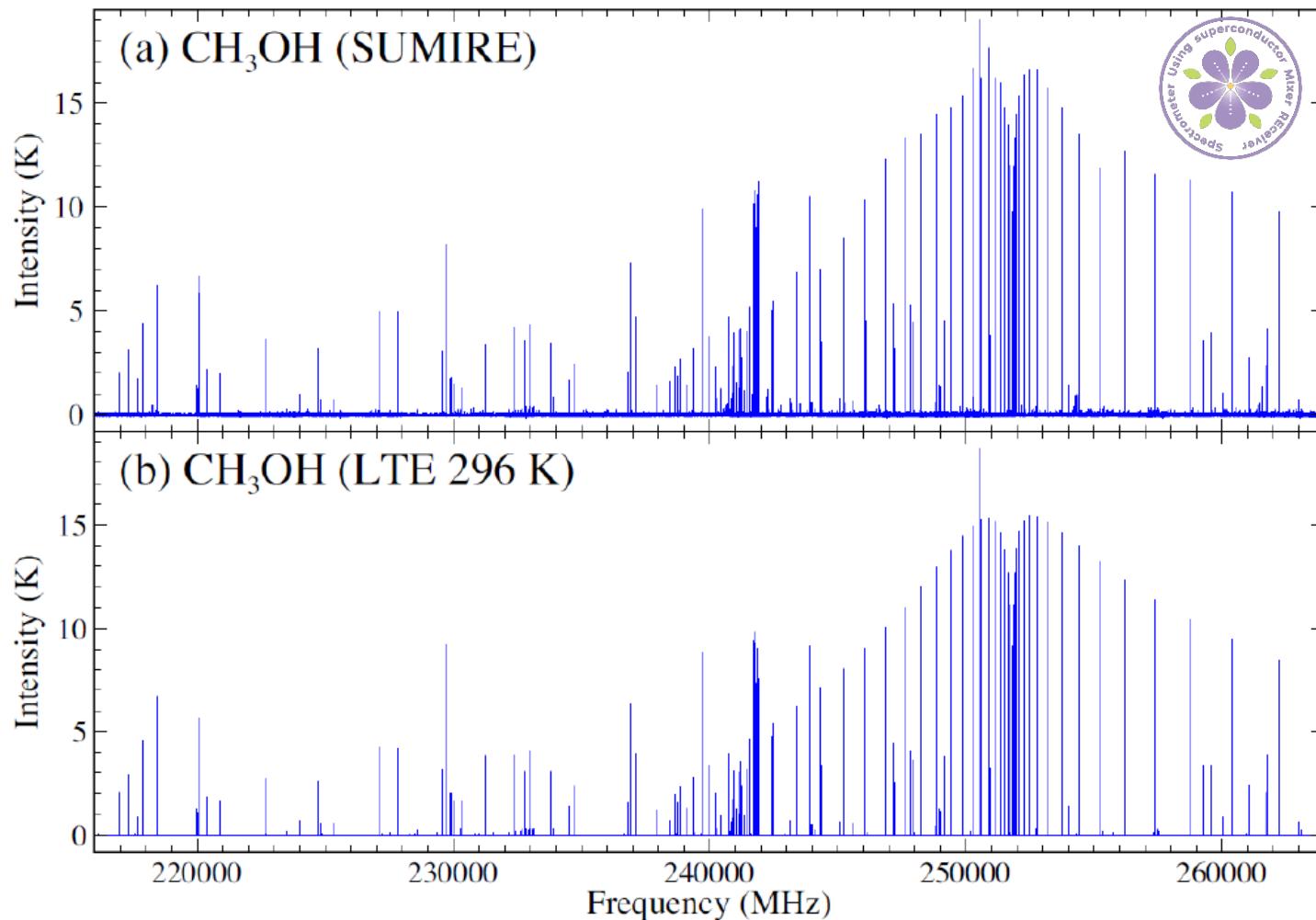
Int. accuracy: 5-10%

Determine
accurate frequency &
absolute intensity ($S\mu^2$)



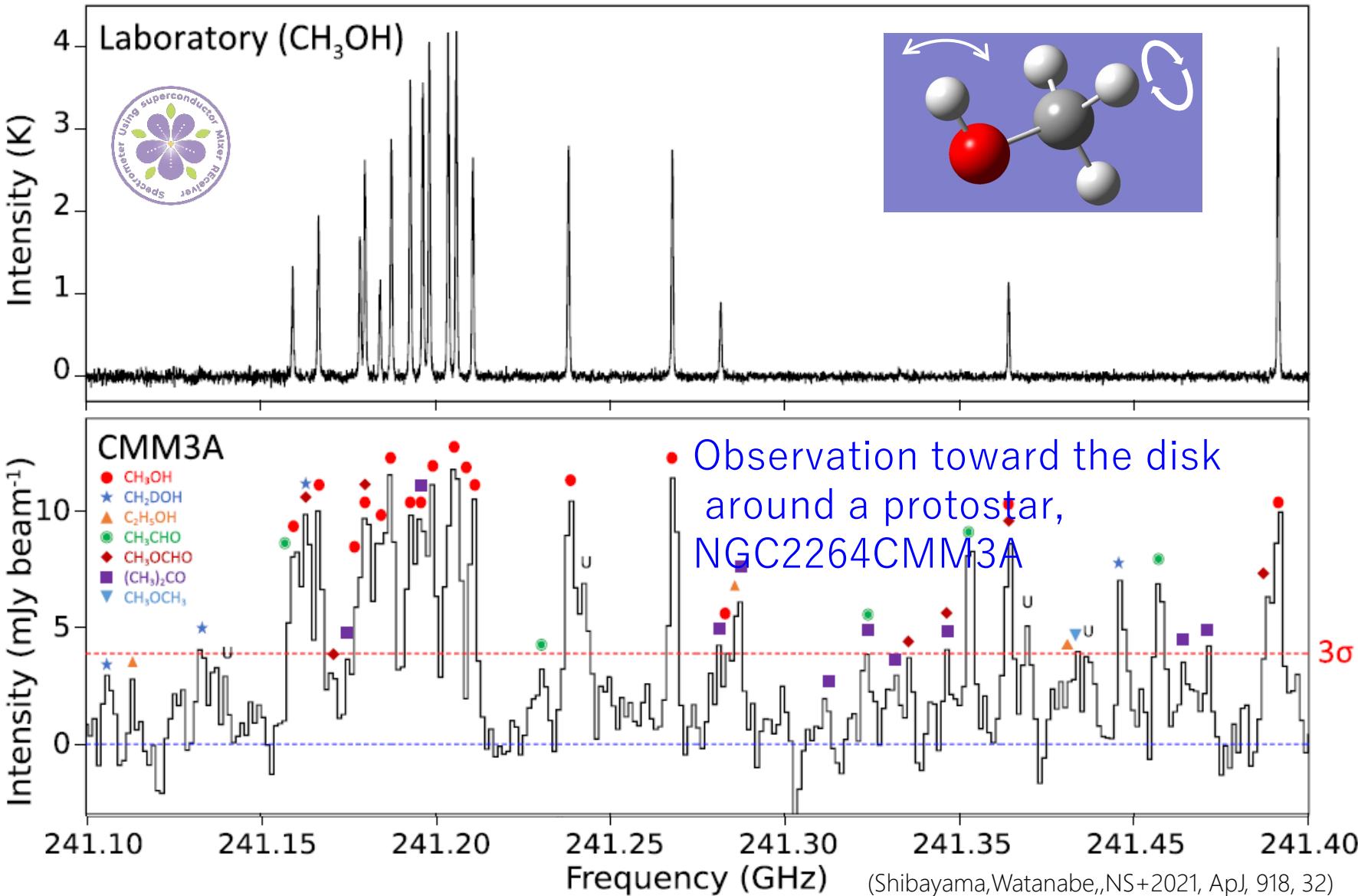


CH₃OH Spectrum taken by SUMIRE





Origin of the “Weeds”: Torsionally Excited Lines ($\nu_t=1$)

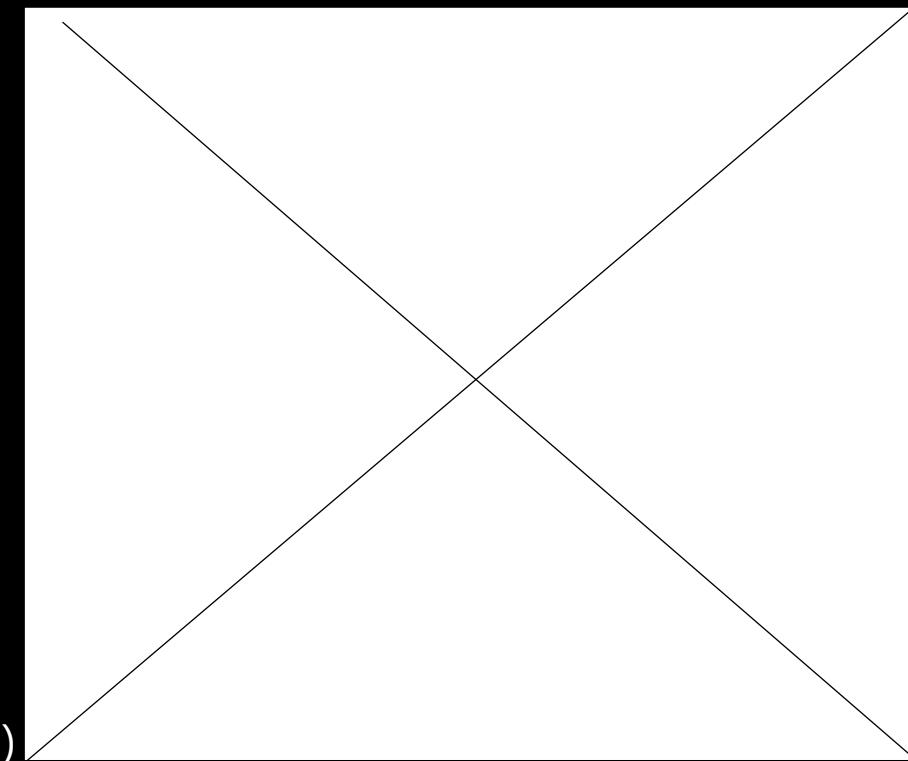
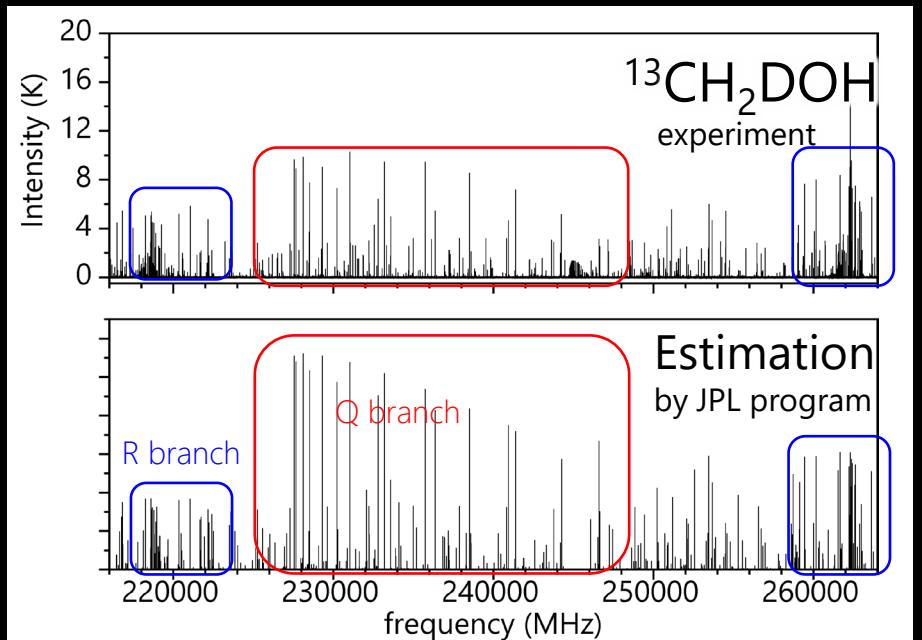




Intensity-Calibrated Spectroscopy



SUMIRE



(Ohno, Y., Oyama, T., ,NS+2022, ApJ, 932, 101)

In JPL(NASA) web site

The intensities were calculated with the first order Fourier term of the dipole from normal methanol. The strongly allowed bands are reasonably well reproduced, but the weaker ones are not as well re-produced. Extreme caution should be used in determining columns (or concentrations) directly from b-type and c-type transitions as significant errors can occur. The a-type transitions should be much more reliable for column determinations.



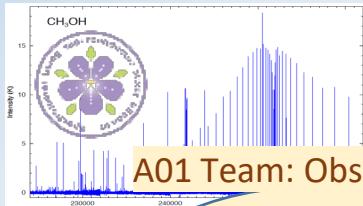
RIKEN-Pioneering Project
「r-EMU: Evolution of
Matter in the Universe」

r-EMU Team: Nucleus

r-EMU Team: Atoms

r-EMU Team: Molecules

THz, Excitation Analysis, Dust evolution



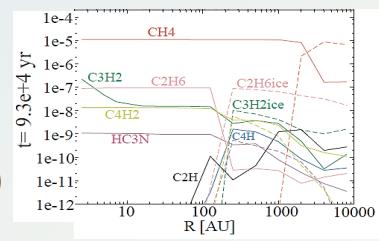
A01 Team: Observation



Cosmic ray ionization
Isotope/Element Ratios
Energetic events
Evolved stars/Dying stars

Quantum chemical calc.

Takayanagi (Saitama-Univ.)
Yamasaki (Hirosaki-Univ.)

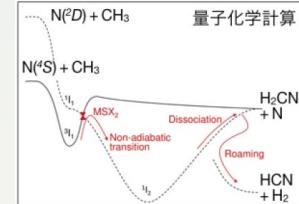


A03 Team: Theory

Chemical network calc.

Physical evolution model.

Aikawa, Y. (Univ. of Tokyo)



Models

Chemical Evolution
Physical Evolution



A02 Team: Analysis

Planetary Science Return Samples

Tachibana, S. (Univ. of Tokyo)

Spectroscopy: in collab. w. NAOJ/UEC
Observation

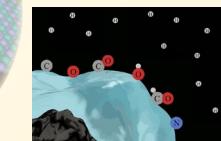
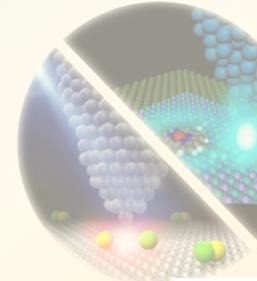
Observations

Sakai, N (RIKEN, CPR)

Distribution
Abundance
Spectroscopy

Next Generation Astrochemistry
JSPS 学術変革領域A
FY2020-2025
PI: Nami Sakai

HAYABUSA 2
Mineralogy, Link to
The Solar System



Gas-Phase Reaction

Branching Ratio
Reaction Rate
Reaction Barrier

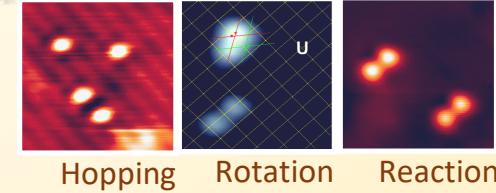
Depletion,
Desorption,
Dissociation,
Dispersion

Surface Reaction

A05 Team: Surface Reaction

Micro: Imada, H., Kim, Y. (RIKEN, CPR)

Macro: Watanabe, N. (Hokkaido Univ.)



A04 Team: Gas-Phase Reaction

Ion - neutral-Atom: Nakano, Y. (Rikkyo Univ.)

Ion - polar-Mol.: Okada, K. (Sophia Univ.)

Ion - isomers: Tanuma, H. (Tokyo Met. Univ.)

(\leftrightarrow Neutral-Neutral: I. Sims (Rennes1, France))

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