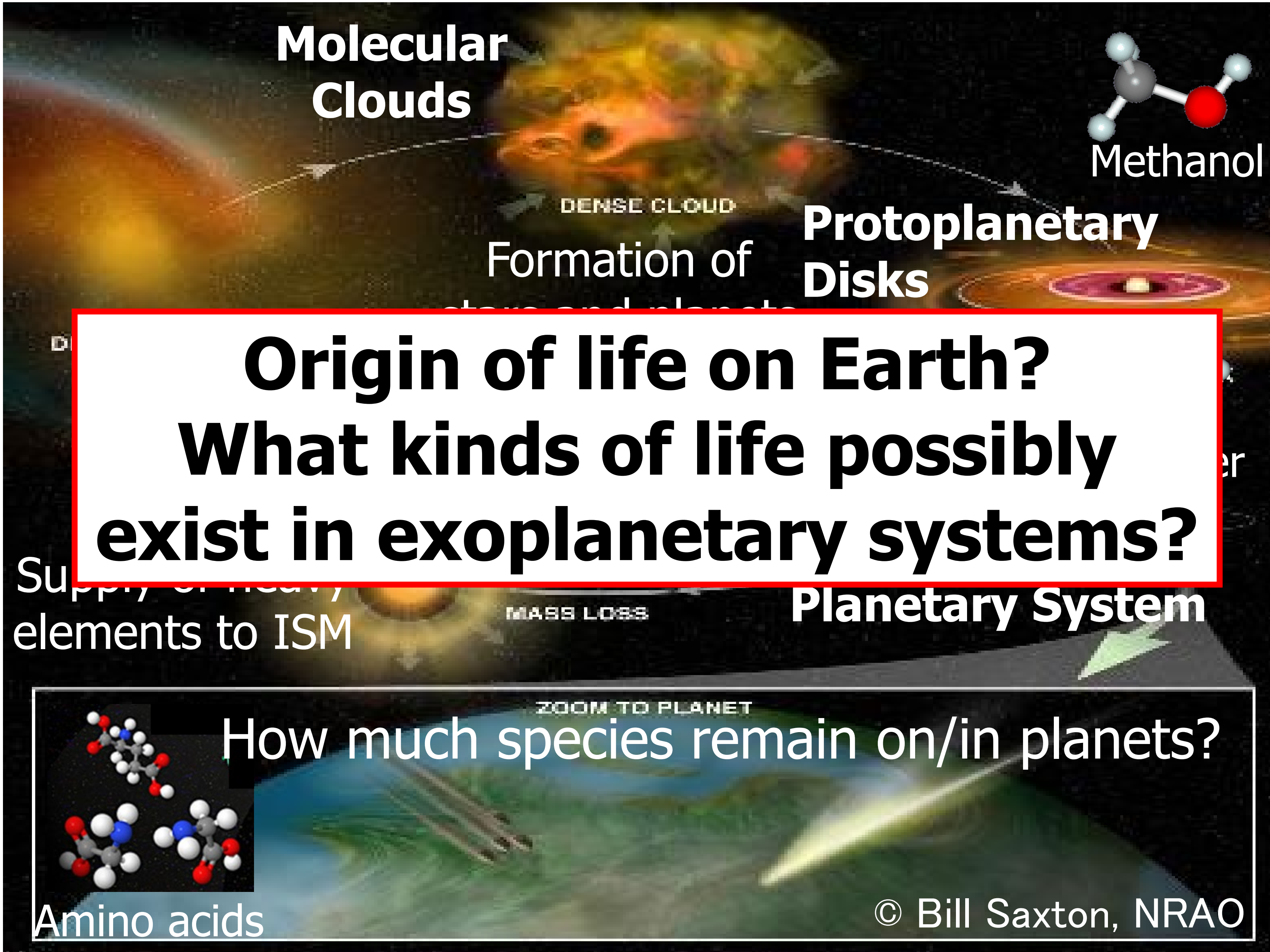
NAOJ Future Planning Symposium 2021
Nov. 9-10, 2021 @ NAOJ

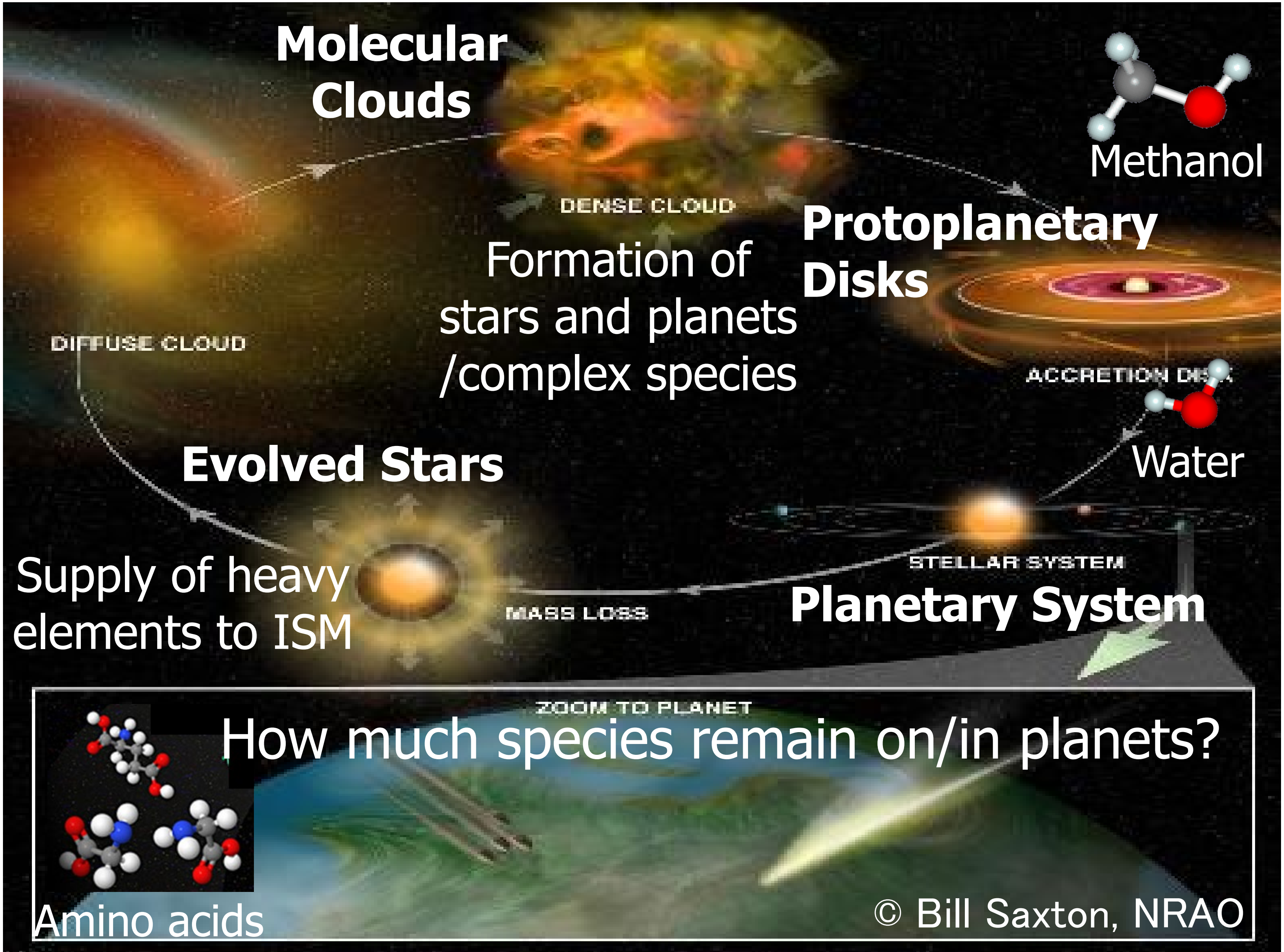
Molecular Evolution

Hideko Nomura
(Division of Science, NAOJ)

Origin of Materials in Planetary Systems



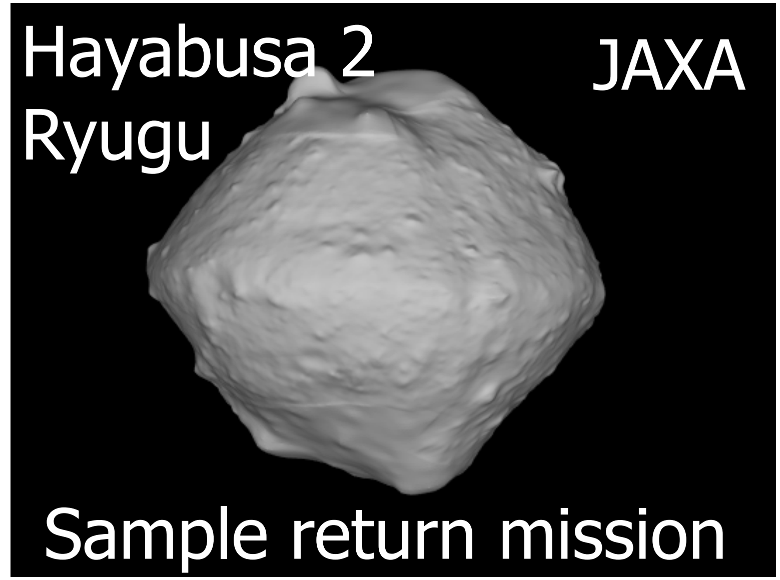
Origin of Materials in Planetary Systems



Solar System Exploration

Amino Acids in Comets & Meteorites

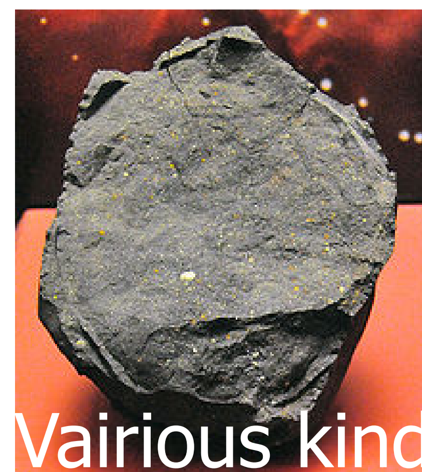
Detection of amino acid, glycine (Elsila et al. 2009)



67P/Churyumov -Gerasimenko

In situ obs. by mass spectrometer (Altwegg et al. 2016)

Murchison meteorites



Vairious kinds of amino acids

Observed Interstellar Molecules

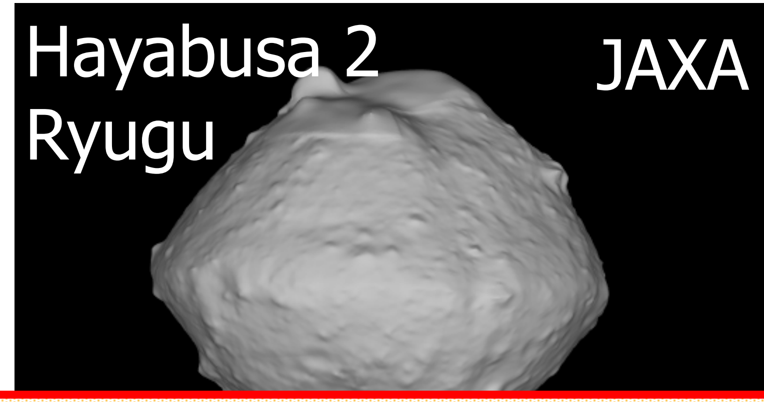
CH+	HCN	H2CO	HC3N	CH3OH	HC5N	HCOOCH3	HC7N
CS	HNC	H2CS	HCOOH	CH3CN	CH3CCH	CH3C3N	HC9N
CO	HCO	H2CN	CH2NH	CH3NC	CH3NH2	CH3COOH	HC11N
CN	OCS	HNCO	CH2CO	CH3SH	CH3CHO	CH2CHCHO	C2H5CN
C2	CH2	HNCS	NH2CN	NH2CHO	CH2CHCN	CH2OHCHO	CH3C4H
CH	**C2H**	**C3H**	**C4H**	**C5H**	**C6H**	H2C6	CH3C5N
CO+	C3	*c*-C3H	c-C3H2	H2C4	c-C2H4O		CH3OCH3
CF+	CO2	C3N	H2C3	HC3NH+	CH2CHOH		C2H5OH
CN-	C2O	C3O	CH2CN	**C5N-**	**C6H-**		CH3CONH2
	C2S	C3S	HCCNC				CH3COCH3
	HCO+	CH3	HNCCC				OHCH2CH2OH
	HOC+	C2H2	CH4				C2H5OCHO
	HCS+	HOCO+	H2COH+	→ **amino acids ?**			
		HCNH+	**C4H-**				**H2COOH?**
		C3N-					

1970 → 1980 → 1995 → 2021

~10 species → ~50 → ~100 → ~270 species

Solar System Exploration

Amino Acids in Comets & Meteorites



How were these organic compounds formed from molecules in space?

Key species: Water & Organics

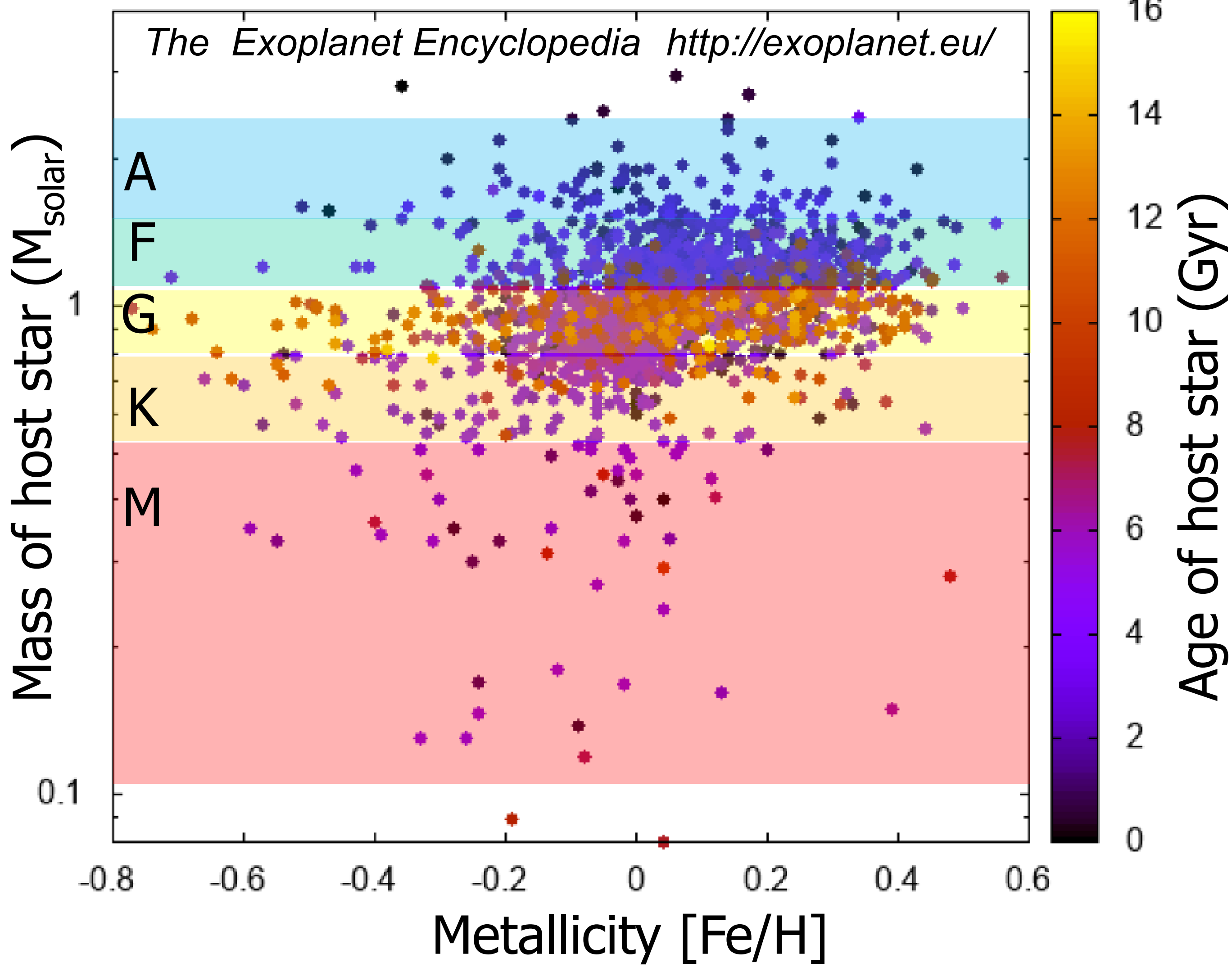
In situ obs. by mass spectrometer
(Altwegg et al. 2016)

of amino acids

Exoplanets: Stellar Type & Age

Sun: 4.6 Gyrs
(z~0.5)

M type stars
(z>0.5)

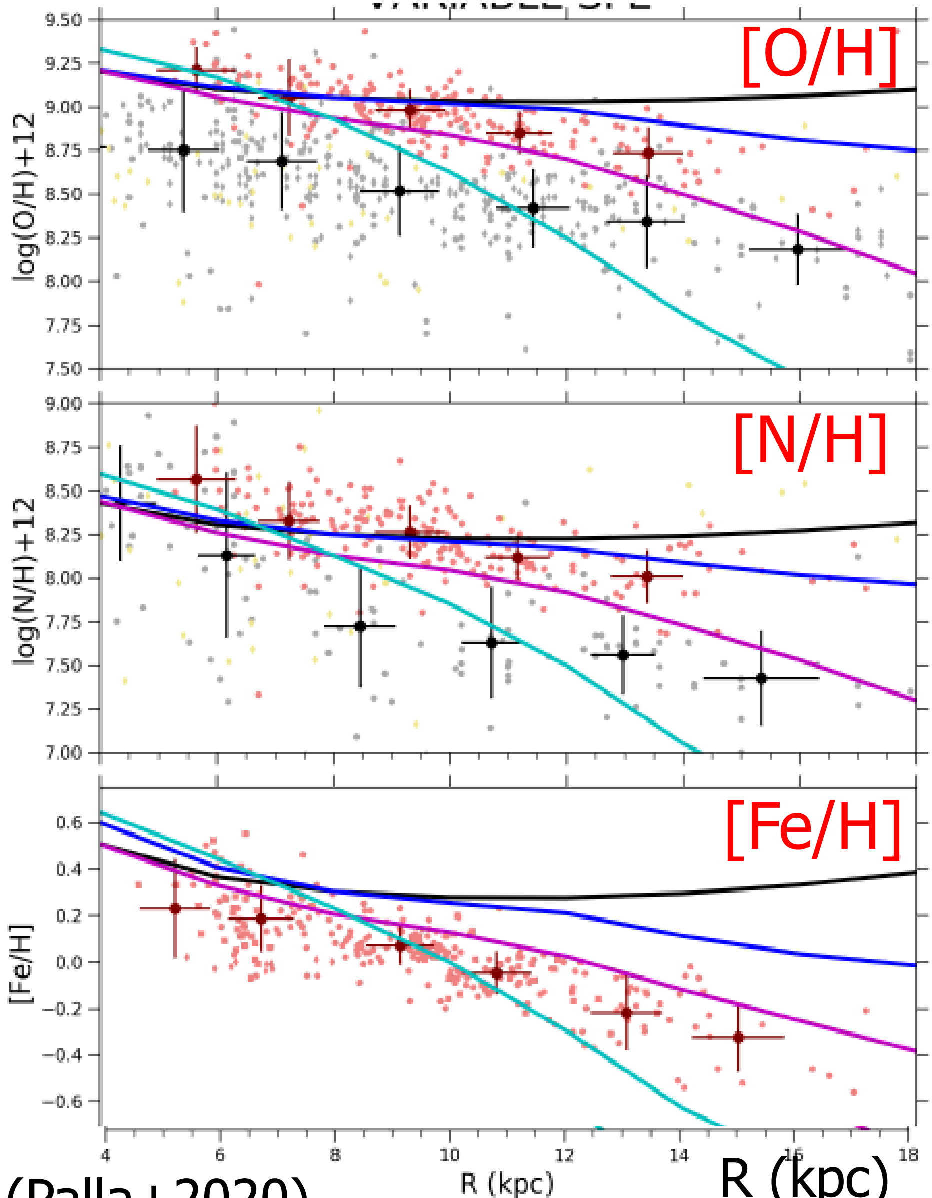


Spectroscopic observations of host stars are important

e.g., Kepler mission, Subaru SSP: Search for Planets like Earth around Late-M Dwarfs: Precise Radial Velocity Survey with IRD

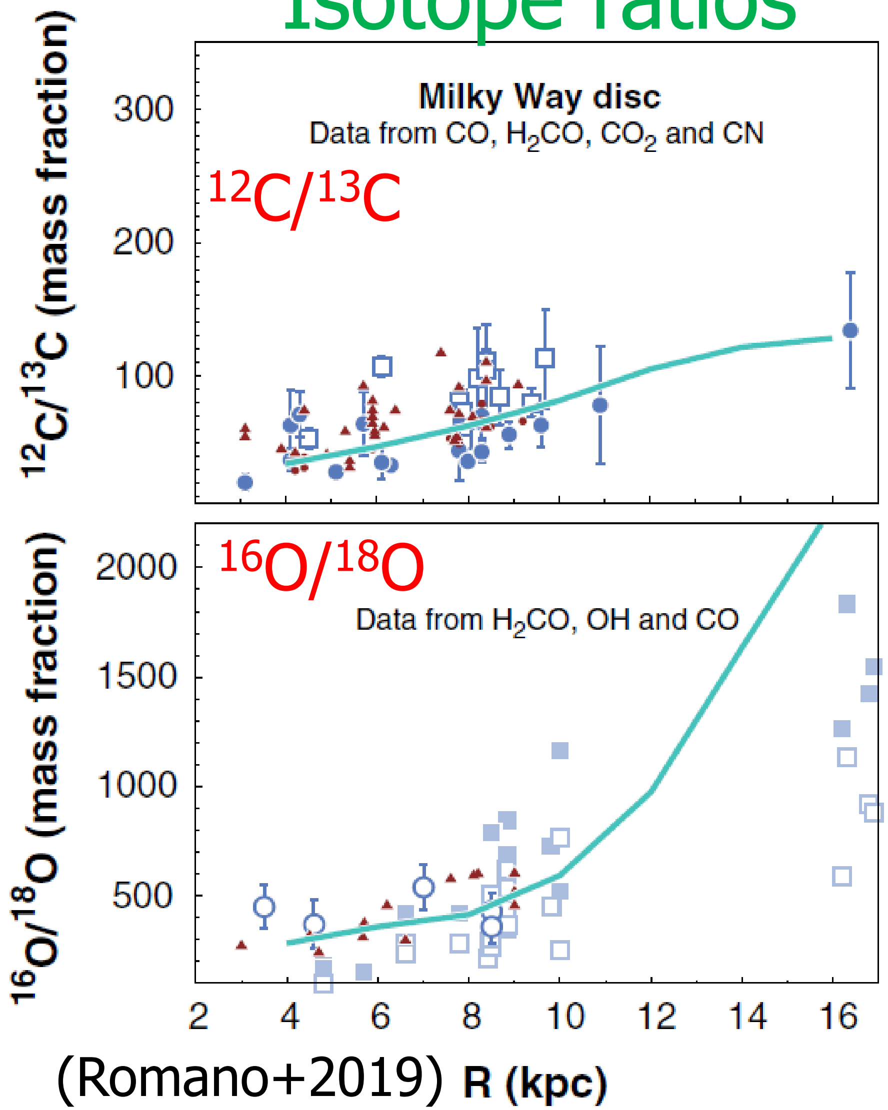
Chemical Evolution in Milky Way

Elemental abundances



(Palla+2020)

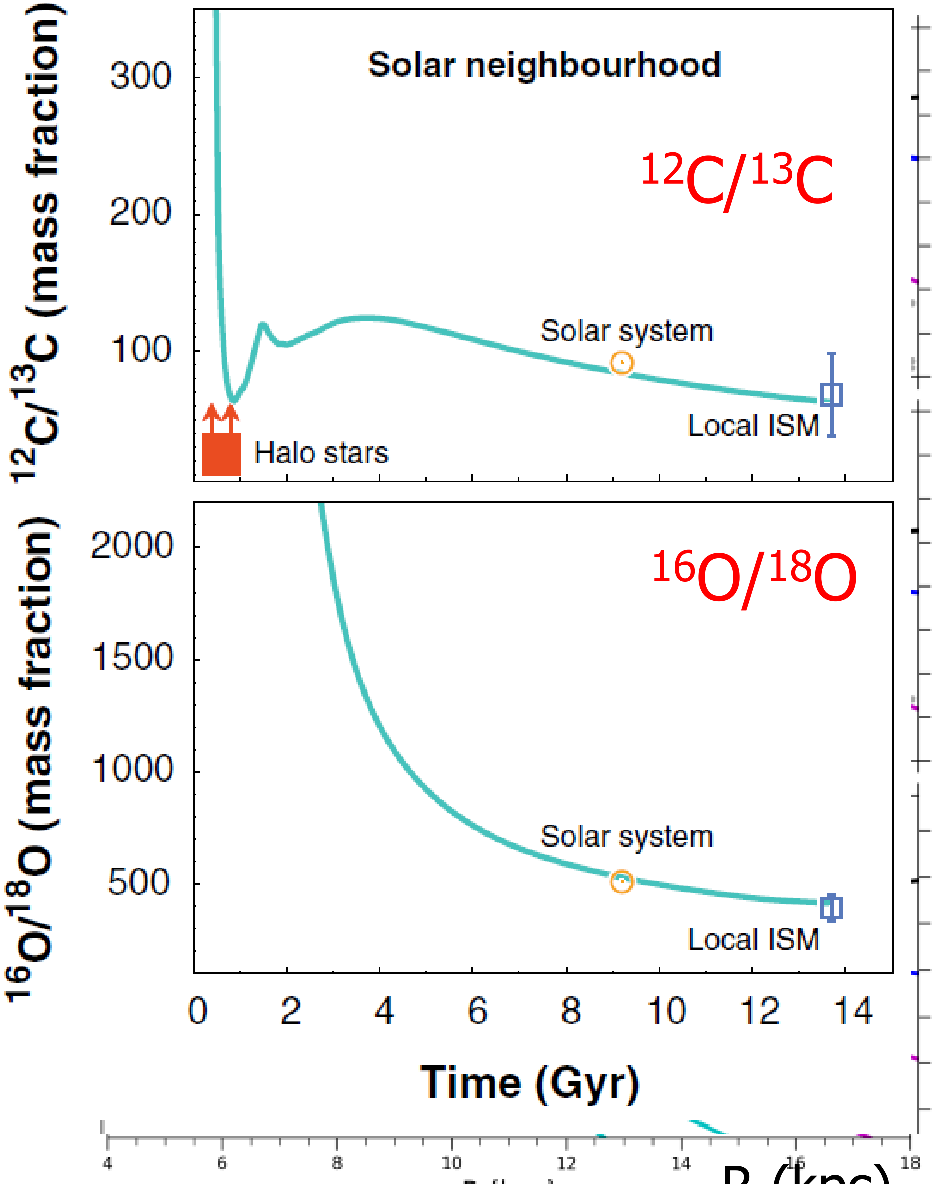
Isotope ratios



(Romano+2019)

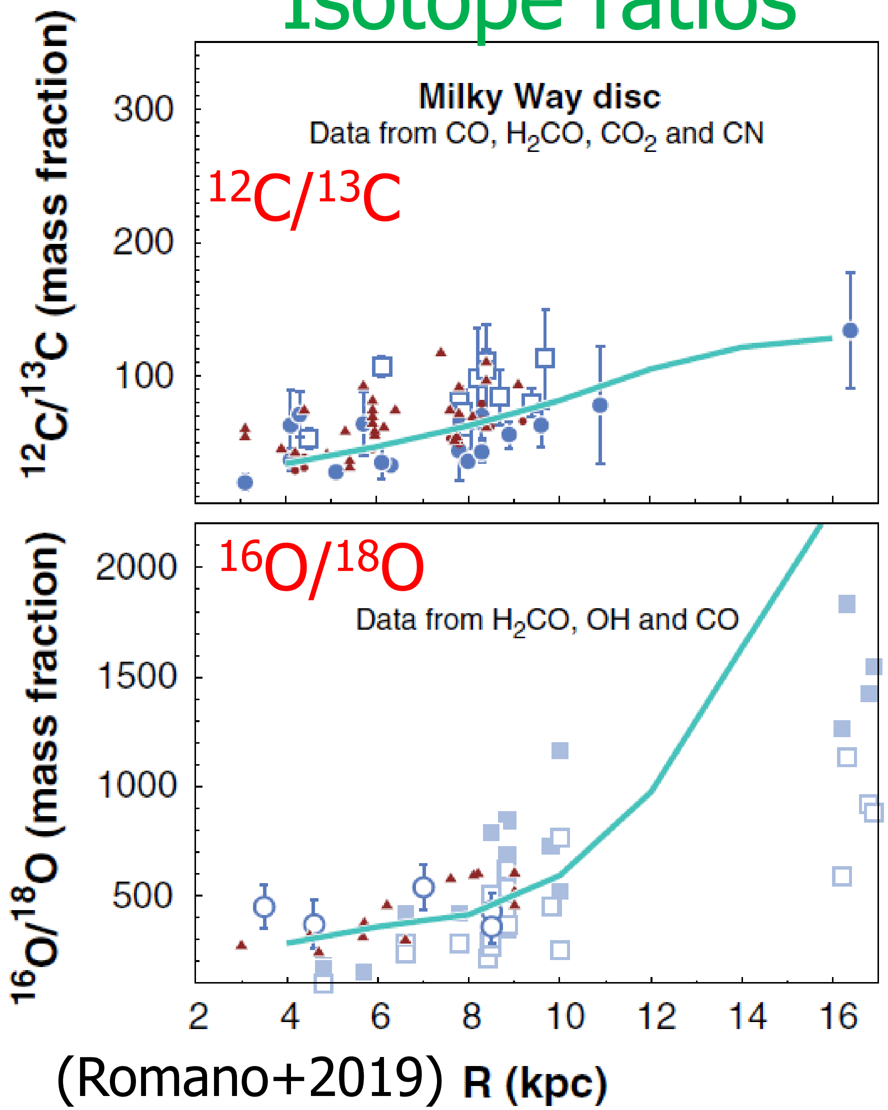
Chemical Evolution in Milky Way

Elemental abundances



(Palla+2020)

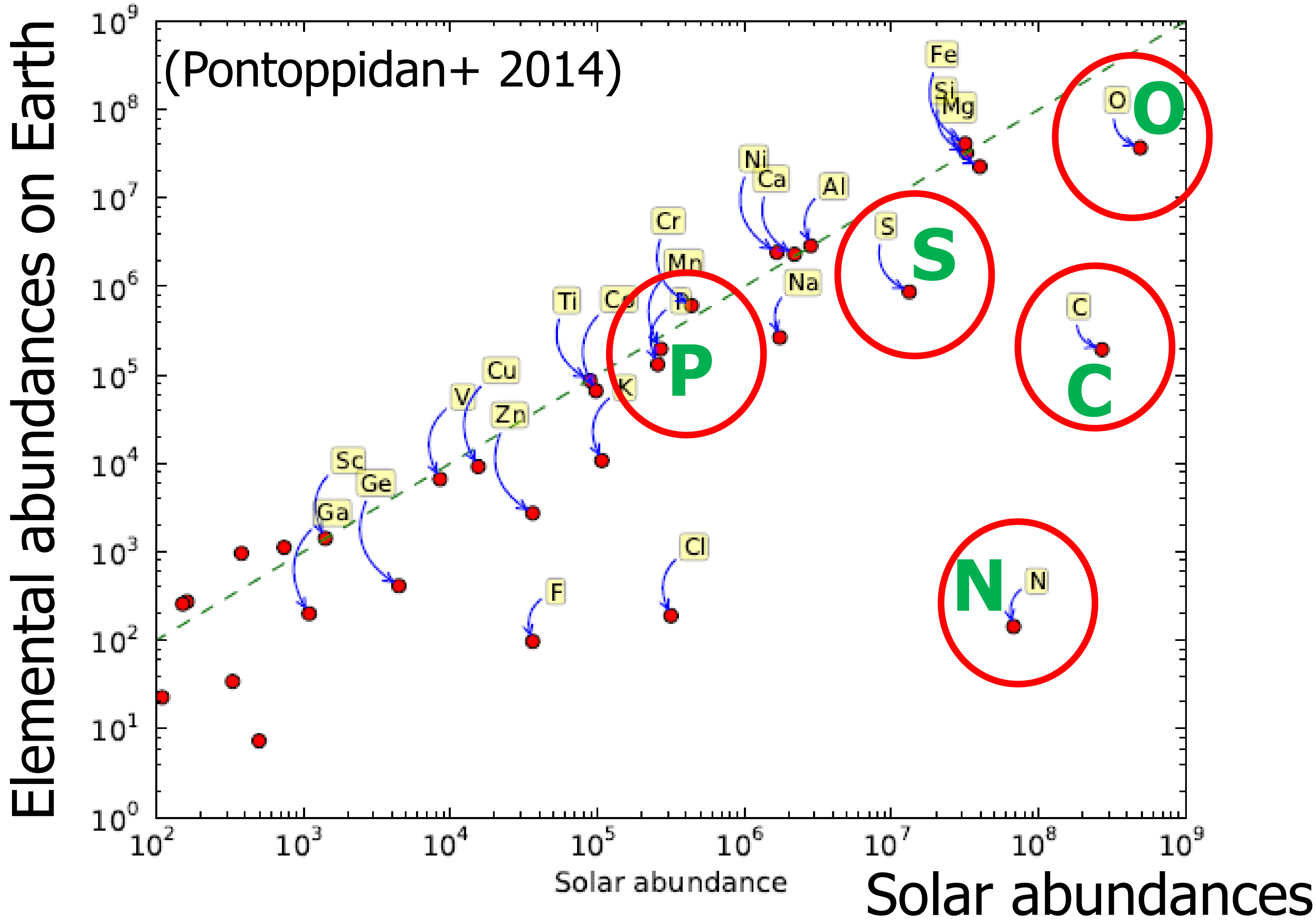
Isotope ratios



(Romano+2019)

→ Kobayashi-san's talk

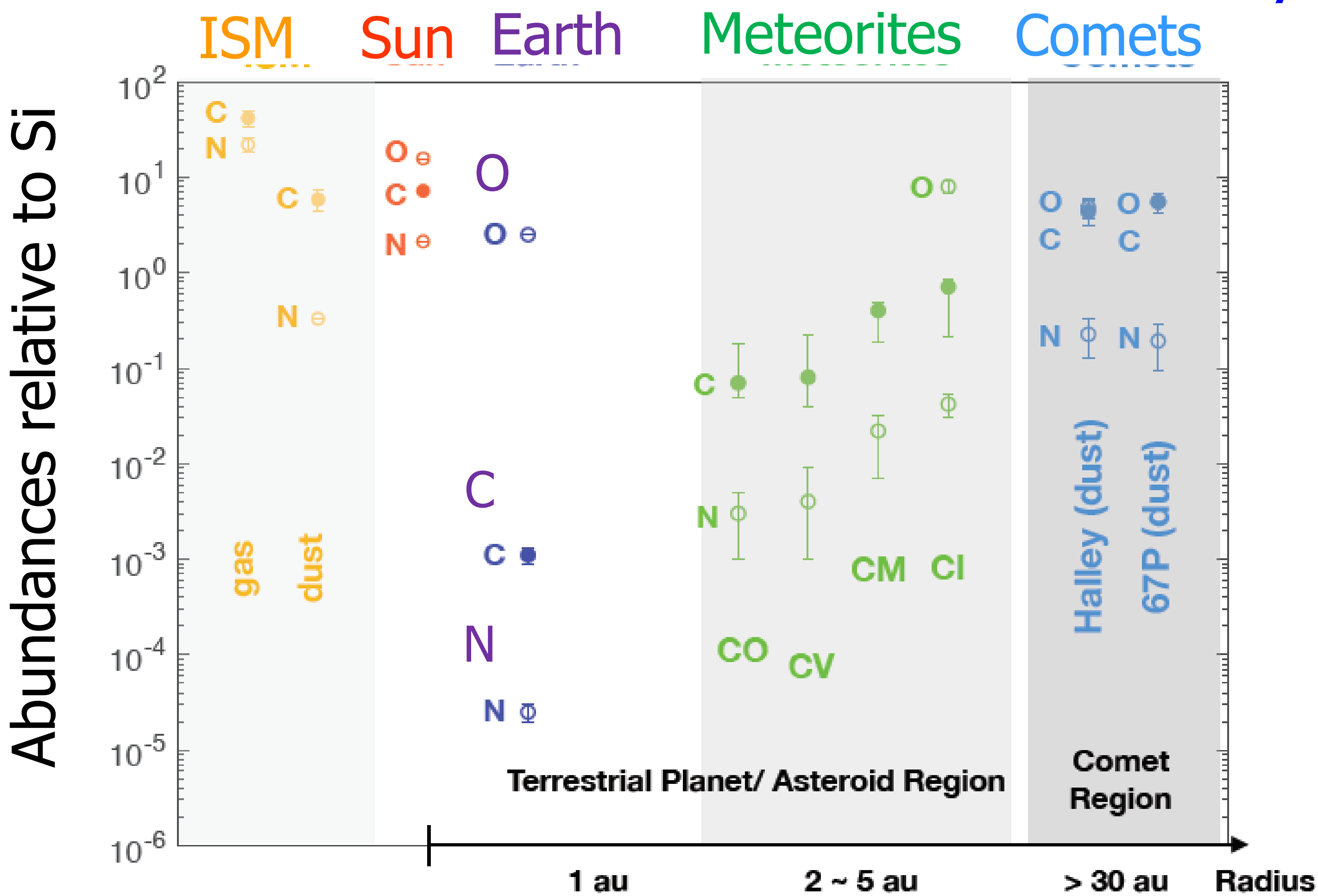
Global vs. Local Elemental Abundances



Nitrogen, carbon, etc. are depleted on Earth

Local Elemental Abundances

Elemental abundances in solids in the Solar system

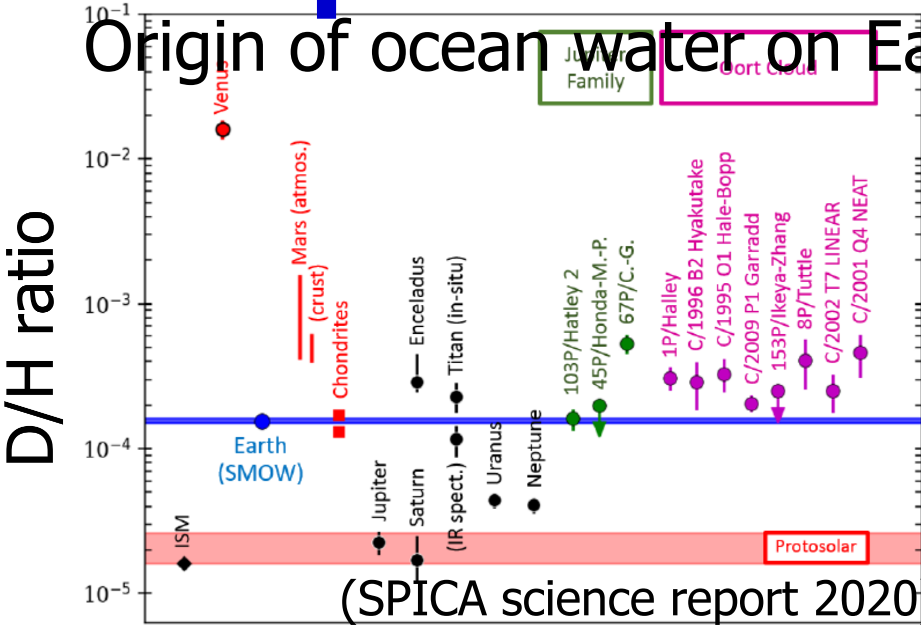


(Lee+10, Pontoppidan+14, Bergin+15, Wei+19)

How do elemental abundances evolve during star and planet formation? How much diversities can arise?

Isotopes : Indicators of Evolution

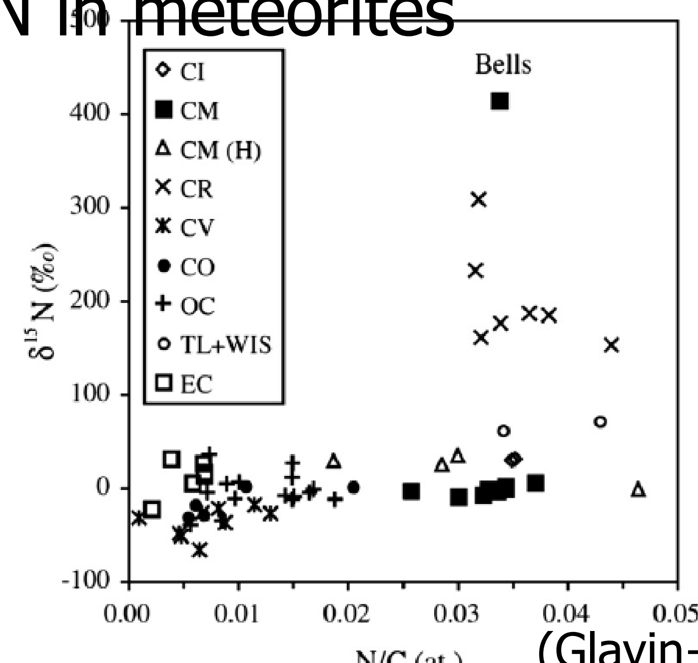
Origin of ocean water on Earth



(SPICA science report 2020)

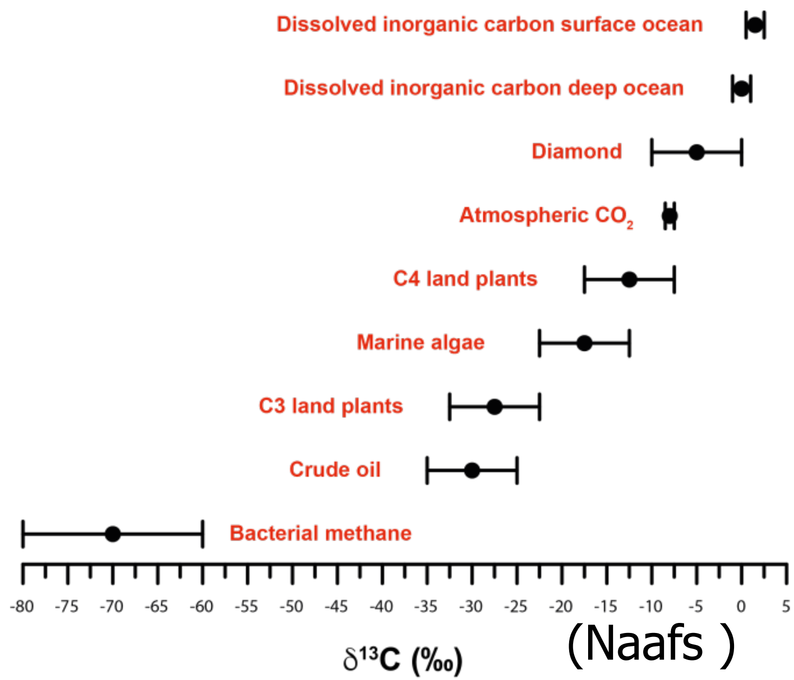
Isotopes can be tracers of origin/evolution of materials.

^{15}N in meteorites



(Glavin+ 2018)

^{13}C in biotic/abiotic components on Earth

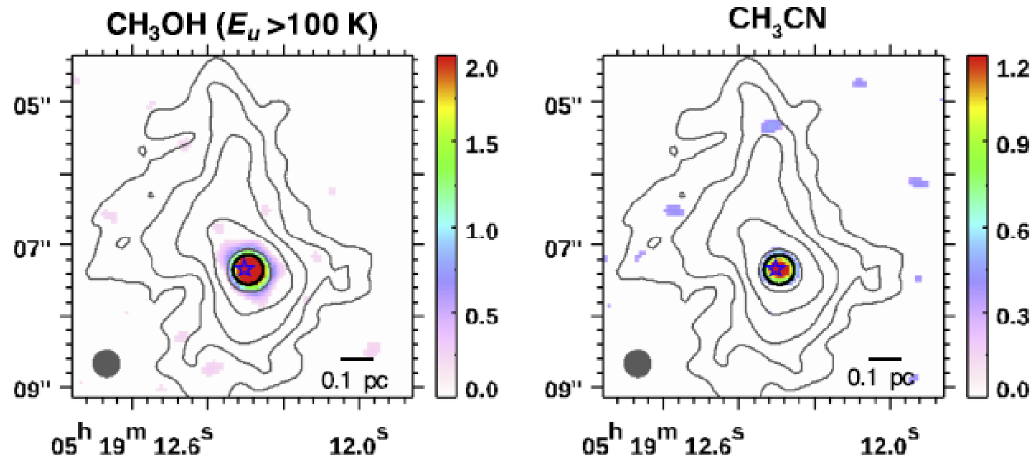


(Naafs)

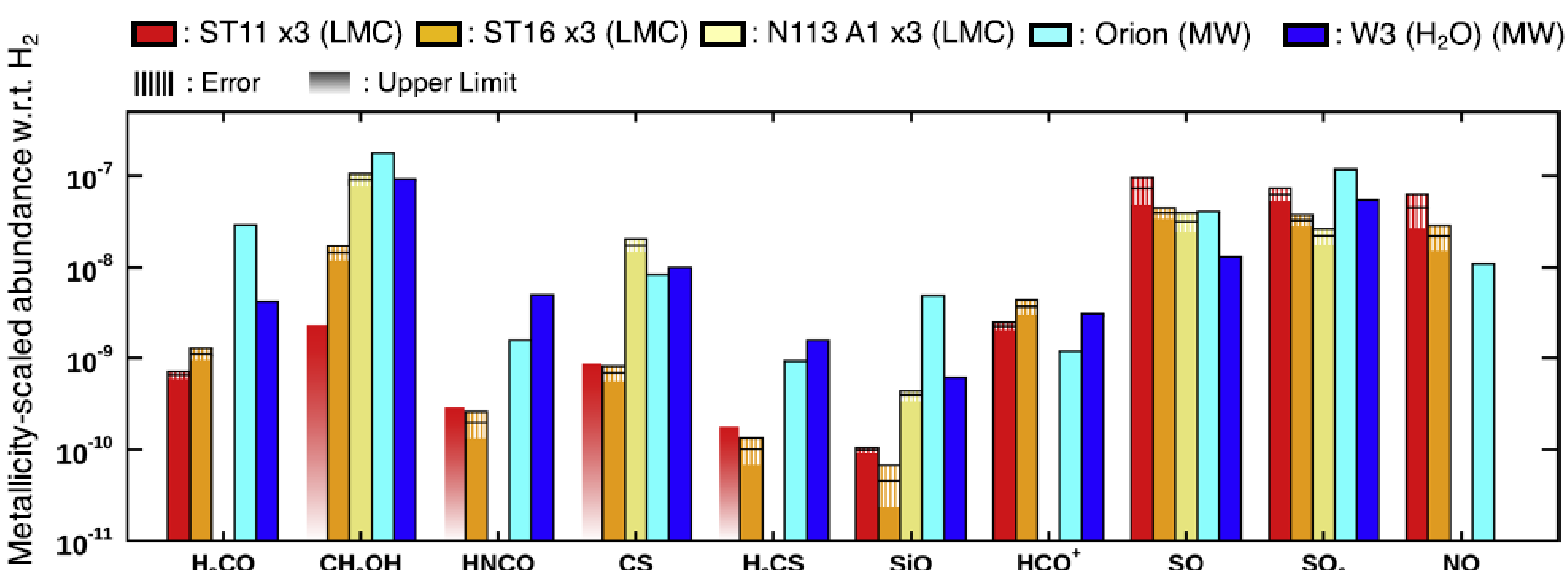
COMs in Low Metallicity

ALMA, Bands 6,7 LMC, ST16

新学術 A paradigm shift by a new integrated theory of star formation



Obs. towards LMC, outer MW → metallicity is not the unique control parameter

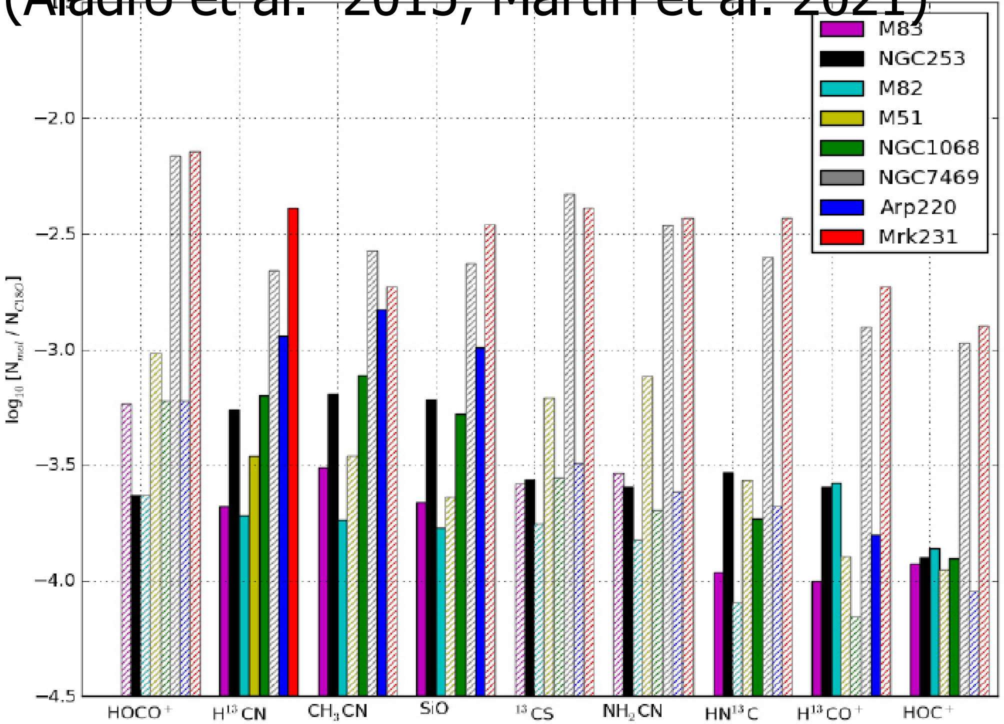


(Shimonishi et al. 2020, 2021)

COMs in Starburst Galaxies/AGNs

(Aladro et al. 2015, Martin et al. 2021)

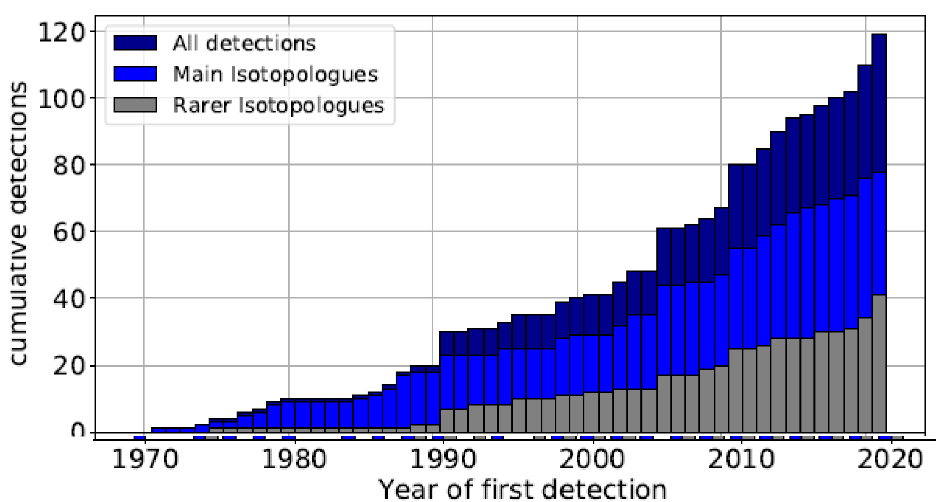
ALMA LP/ ALCHEMI



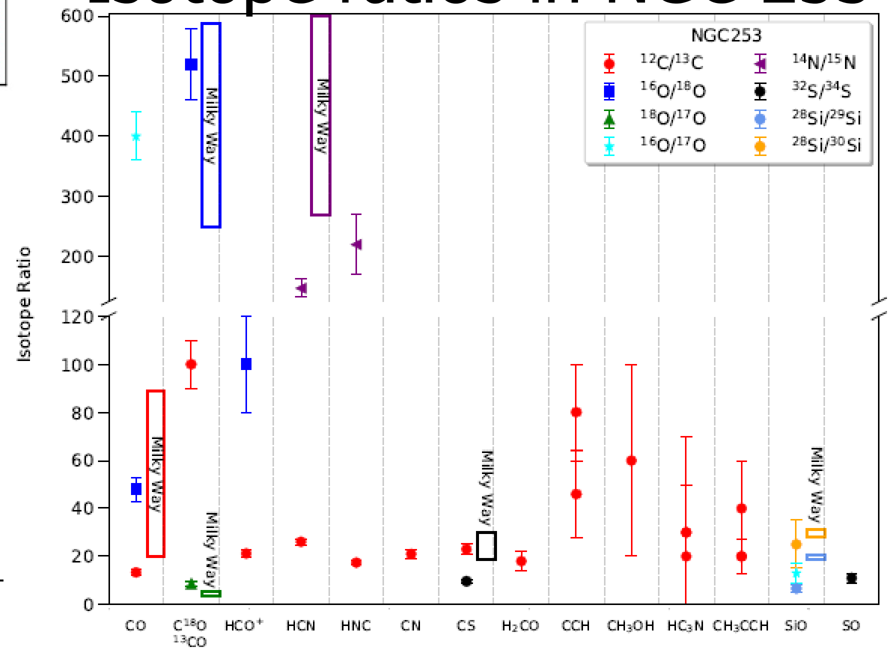
Strong UV, X-ray, cosmic-ray, mechanical heating

(cf. Galactic Center)

→ Variety in chemistry



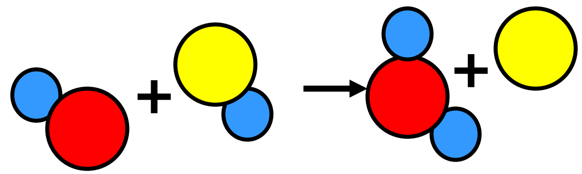
Isotope ratios in NGC 253



Chemistry in the Molecular Clouds

Gas-phase reactions

Neutral-Neutral Reactions

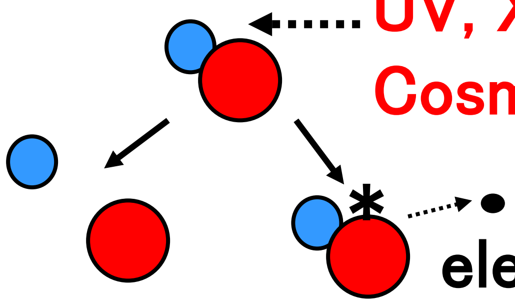


＊Effective on Earth

High activation energies→ Inefficient at low temp. (~10K)

Cosmic-ray Induced Reactions, Photoreactions

UV, X−rays, Cosmic rays



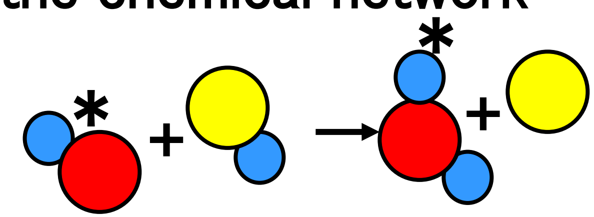
electrons

＊Radicals are abundant

\+

Ion-Neutral Reactions

＊More than half reactions in the chemical network

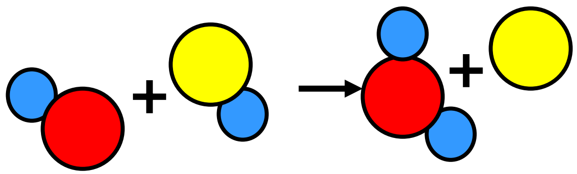


\+ Ion-electron recombination

Chemistry in the Molecular Clouds

Gas-phase reactions

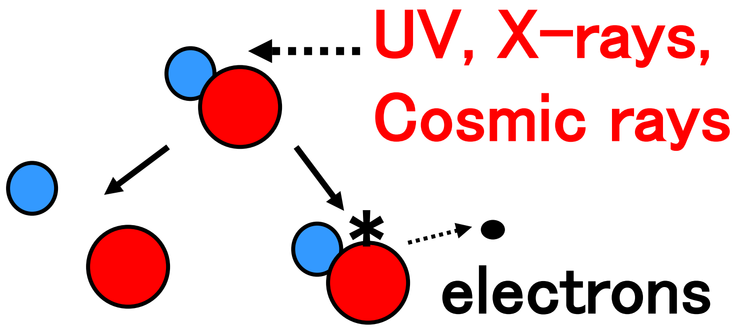
Neutral-Neutral Reactions



＊Effective on Earth

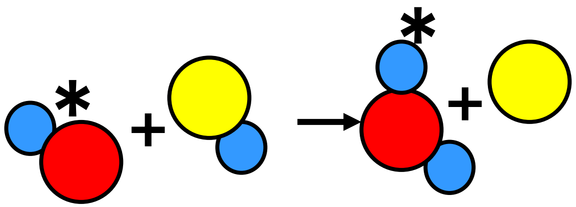
Chemical properties of molecules
⇔ physical properties of objects
(temp. of gas & dust, UV, cosmic rays, X-rays)

Photoreactions



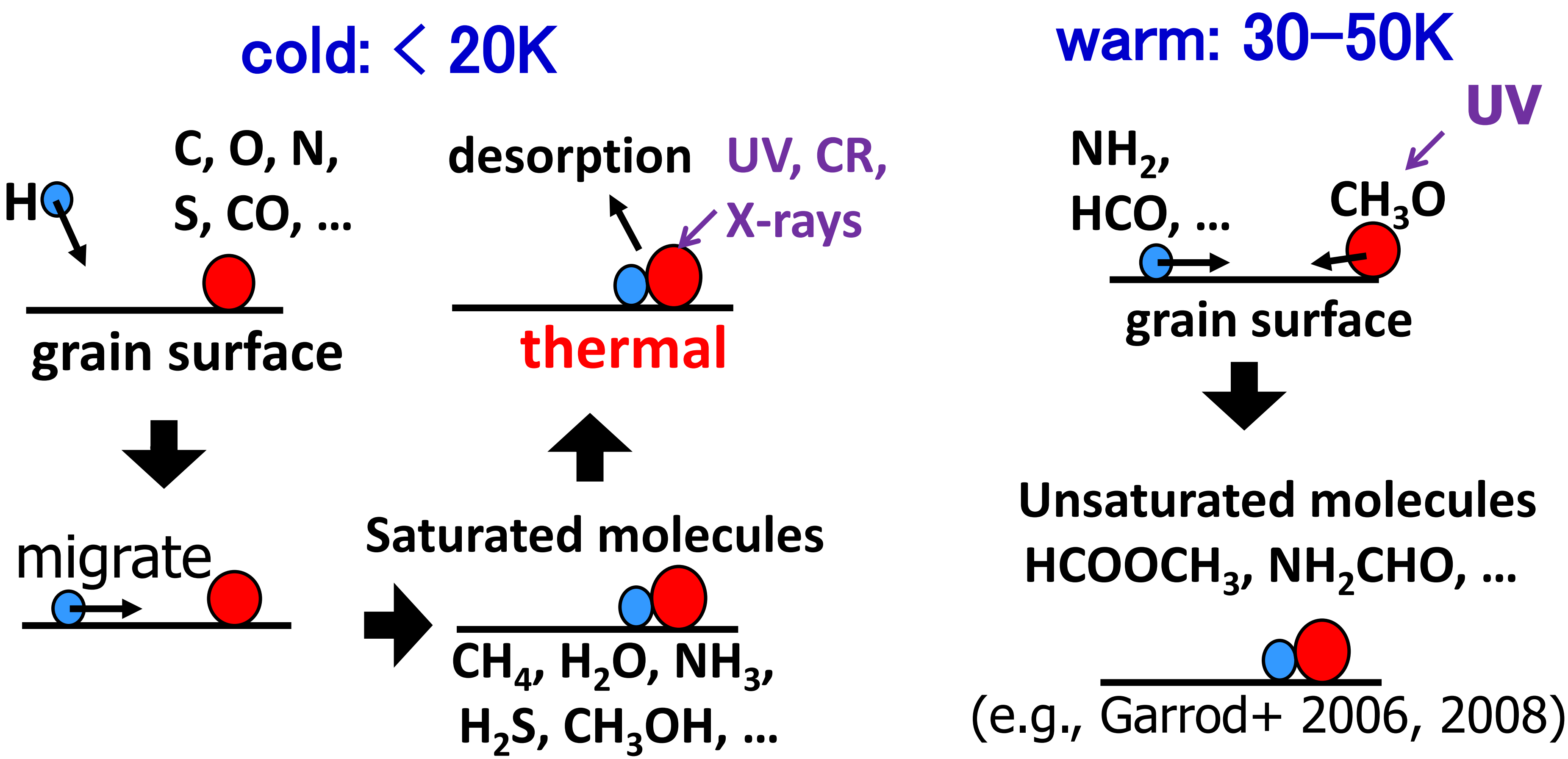
＊Radicals are abundant

＊More than half reactions in the chemical network



+ Ion-electron recombination

Complex Molecule Fomration on Grain Surface



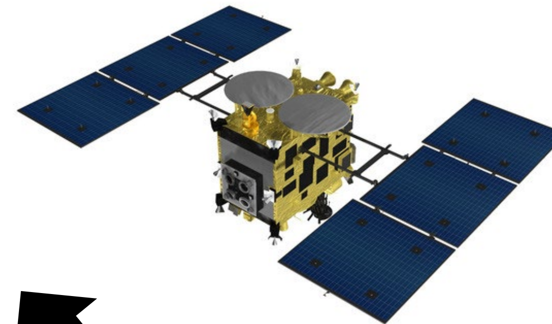
Complex molecules are formed on grains

More complex molecules on warm grains

To Understand Material Evolution

学術変革　Next Generation Astrochemistry

Observation



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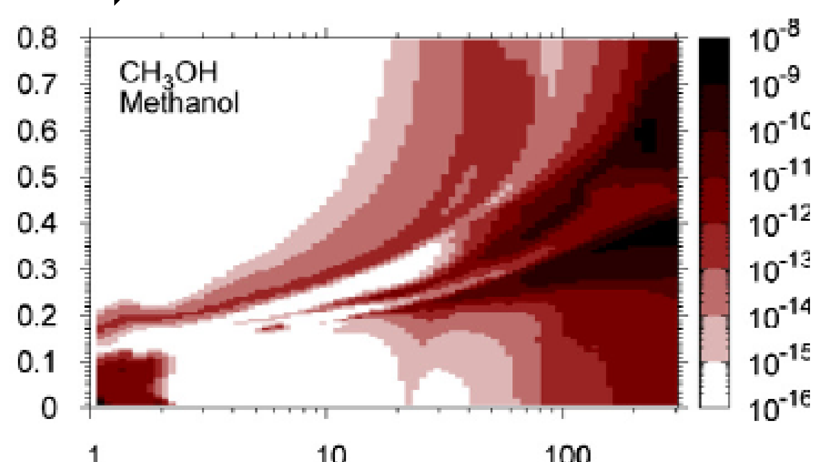
Microprocess (Laboratory, Theory)

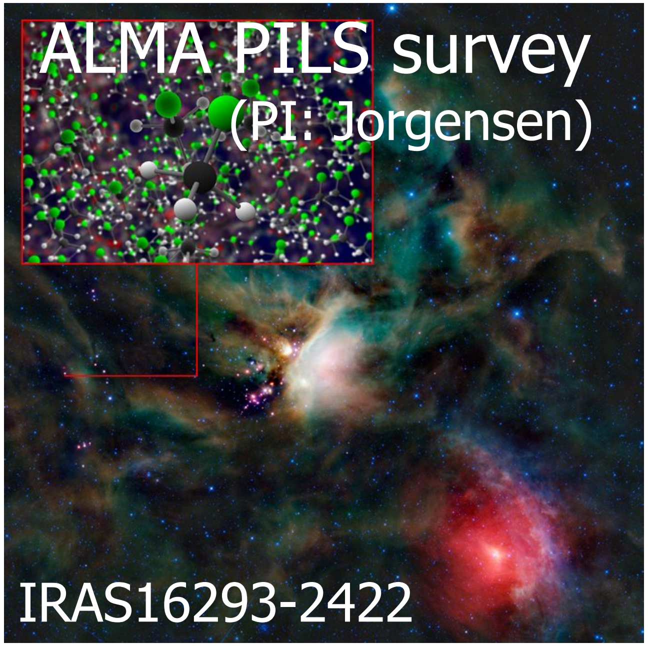
- Gas-phase chemistry (nonthermal chemistry, UV, X-rays, cosmic rays)
- Grain surface chemistry
- Spectroscopy

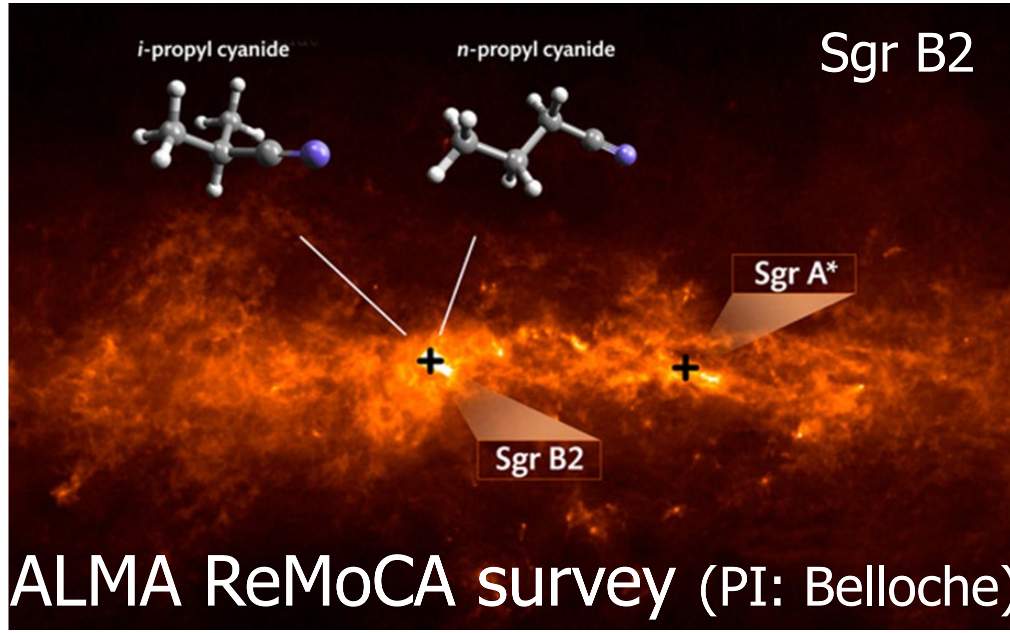
Model

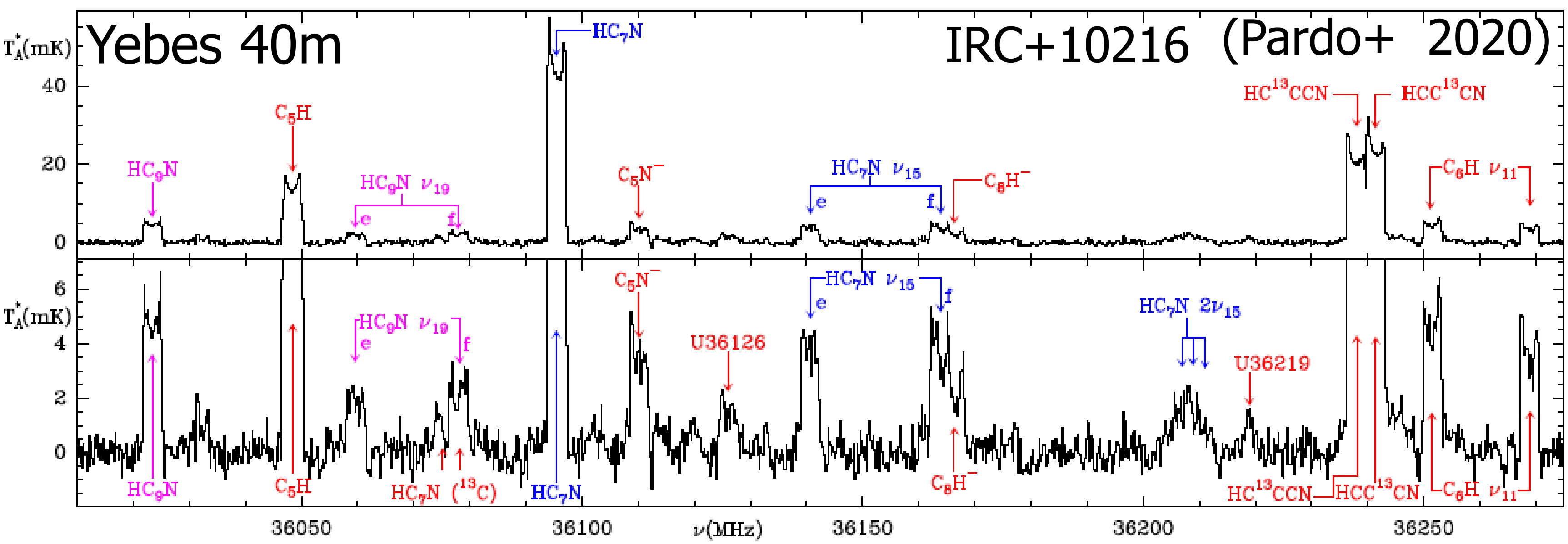


(Walsh+2014)

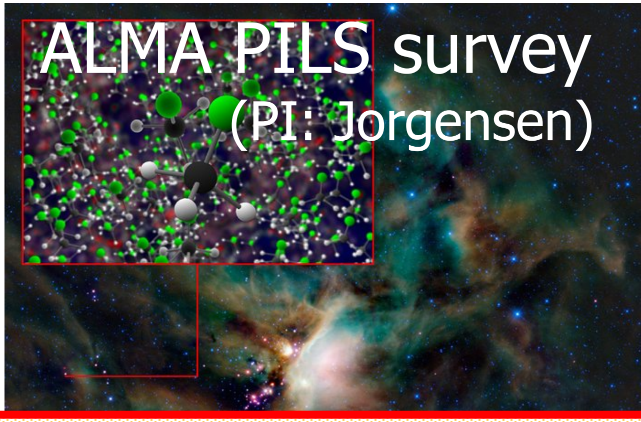
More COMs in Interstellar Clouds

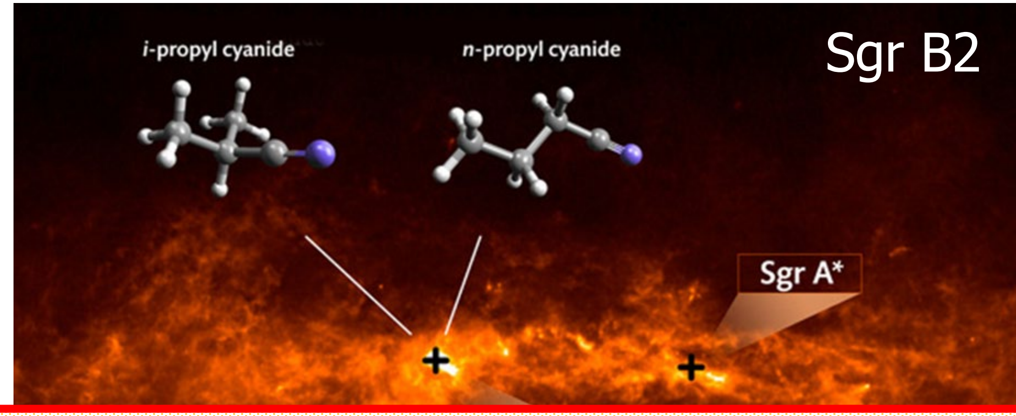






More COMs in Interstellar Clouds

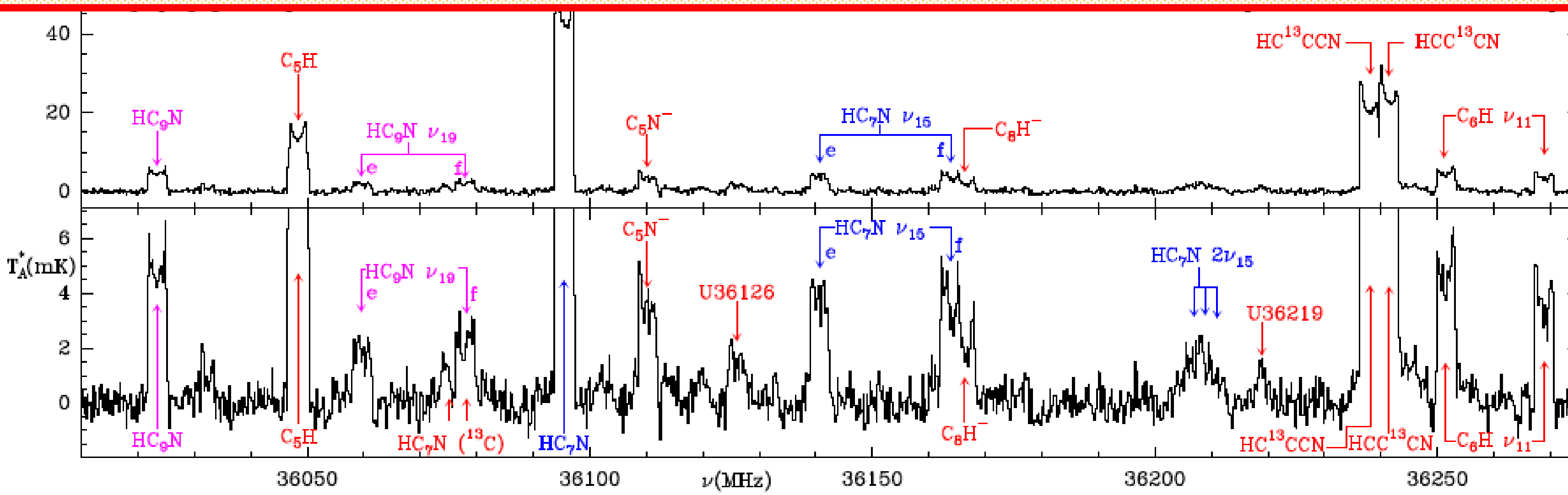




ALMA, GBT, Yebes 40m, etc.

Broad band receiver x laboratory spectroscopy

→ discover 28 molecules this year!



From Molecular Clouds to Planetary Systems

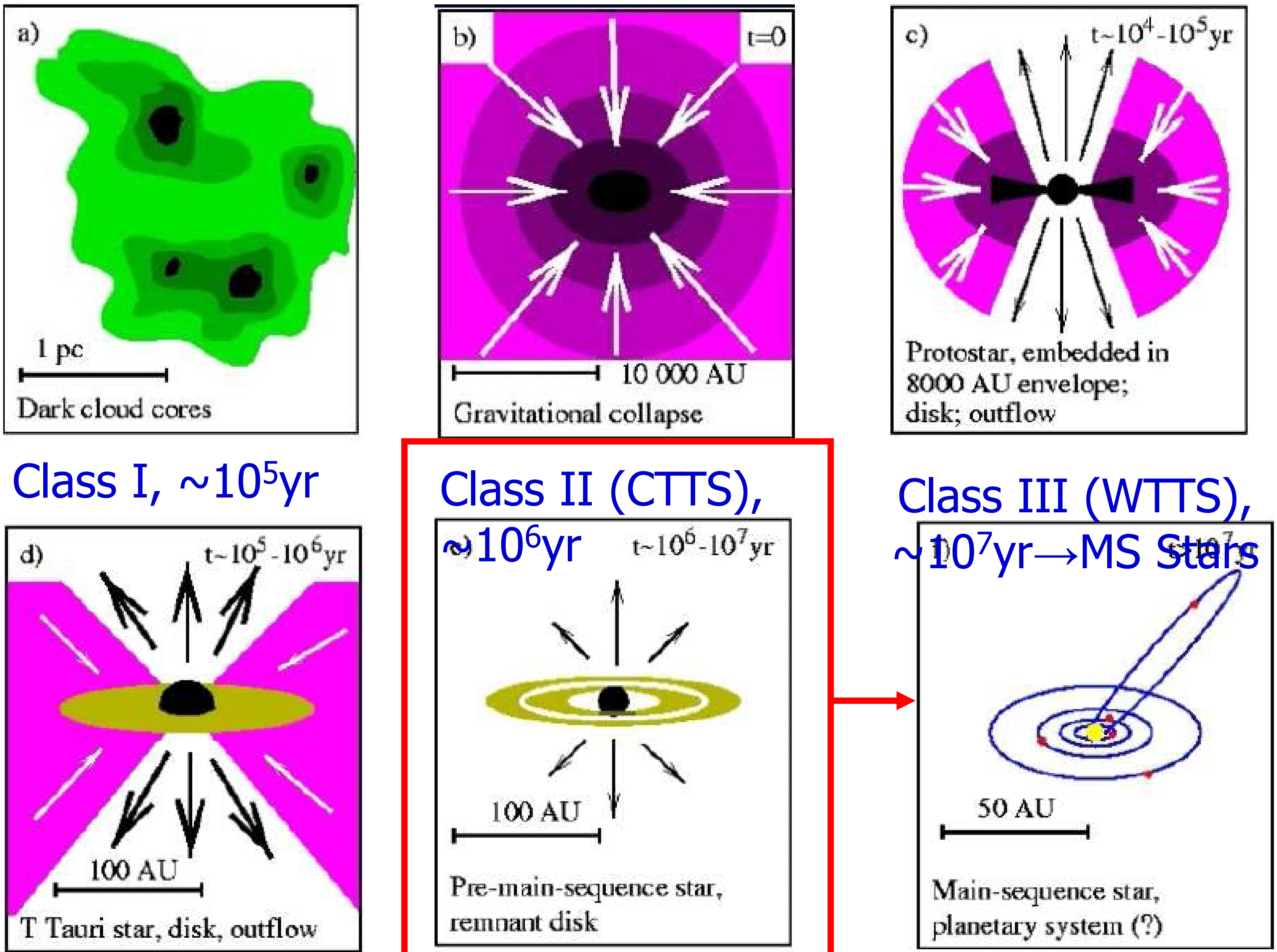
Molecular Cloud Cores, ~10^{6}yr

Class 0, ~10^{4}yr

Class I, ~10^{5}yr

Class II (CTTS), ~10^{6}yr

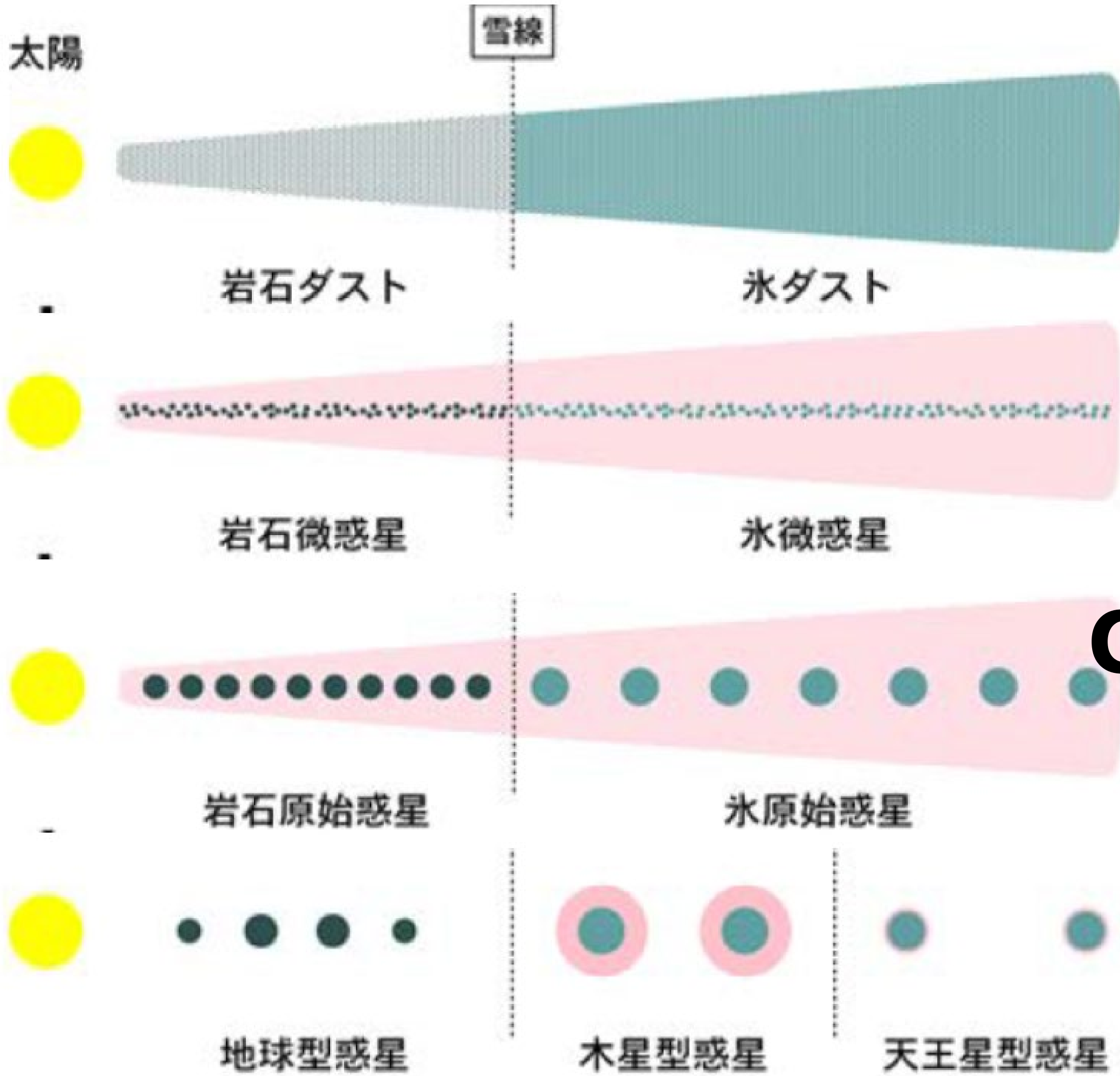
Class III (WTTS), ~10^{7}yr→MS Stars



Hogerheijde 1998, after Shu et al. 1987

From protoplanetary disk to planets

(e.g., Hayashi et al. 1985)



Dust growth & settling

↓

Planetisimal formation

↓

Collisional growth of planetisimals

↓

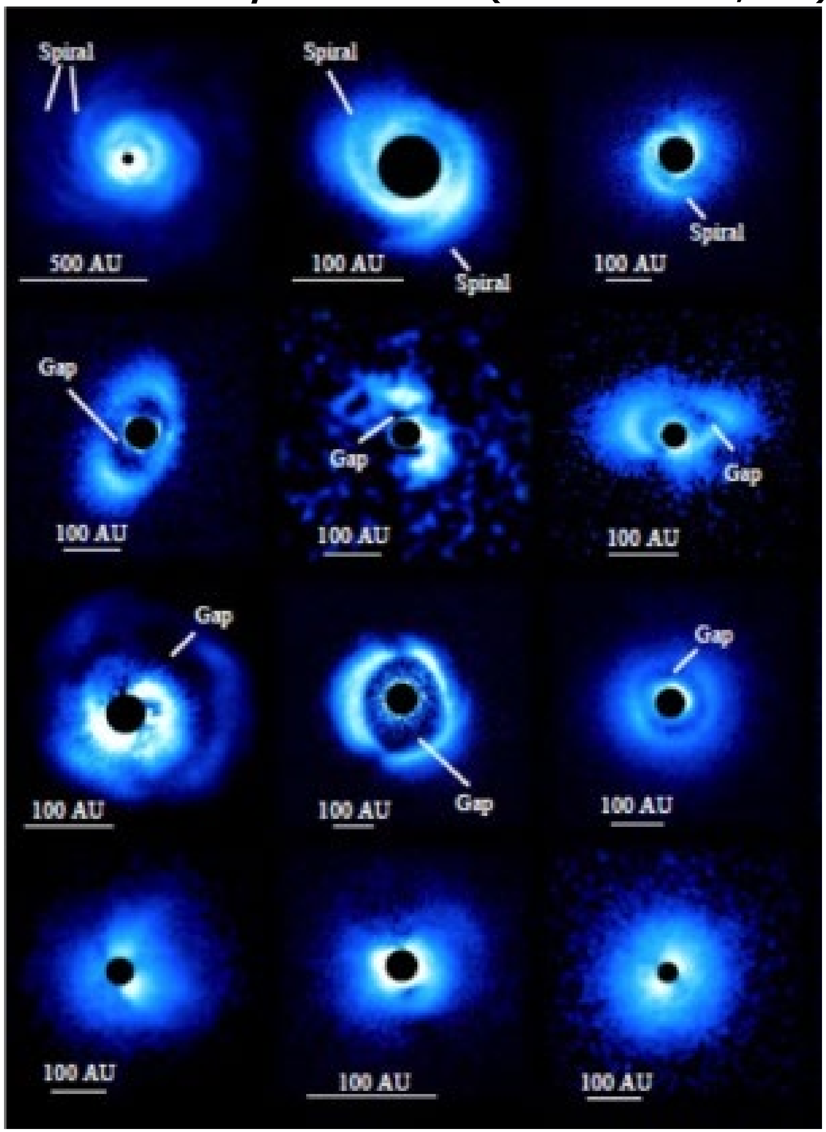
Planet formation

↓

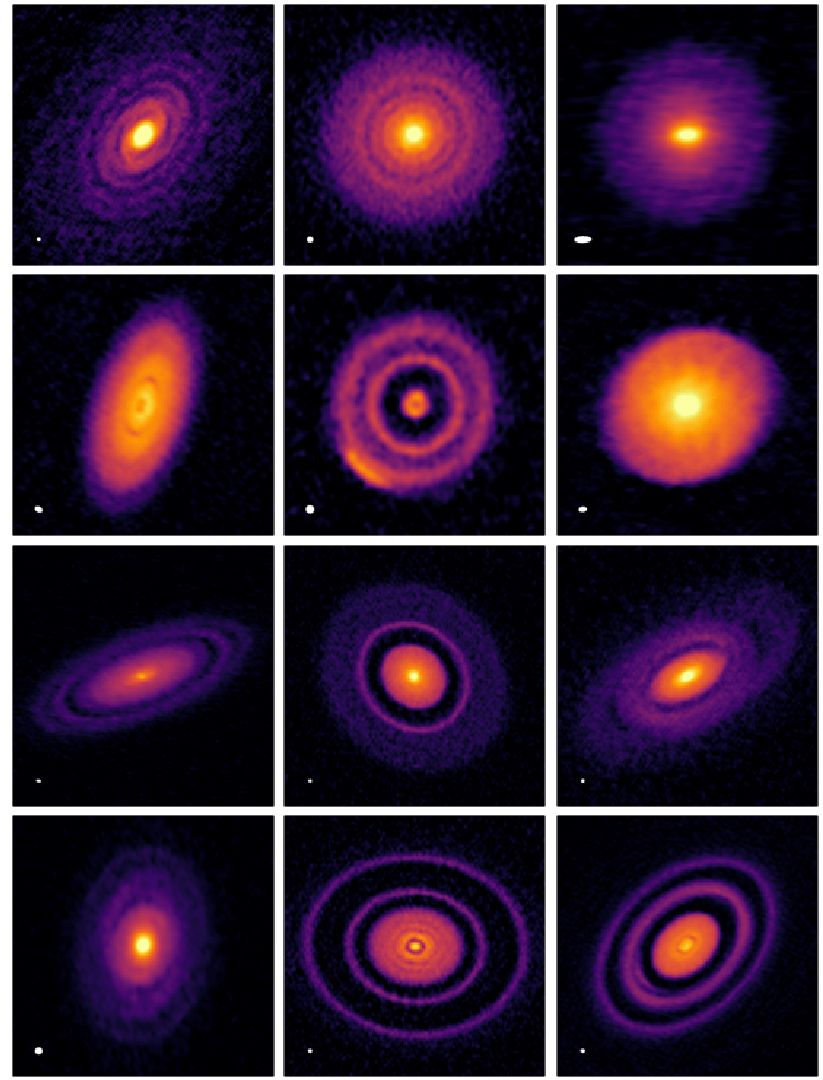
Dispersal of gas

High Res. Obs. of Dust in Disks

Subaru SSP/SEEDS (PI: Tamura, M.)



ALMA LP/DSHARP (Andrews+ 2018)



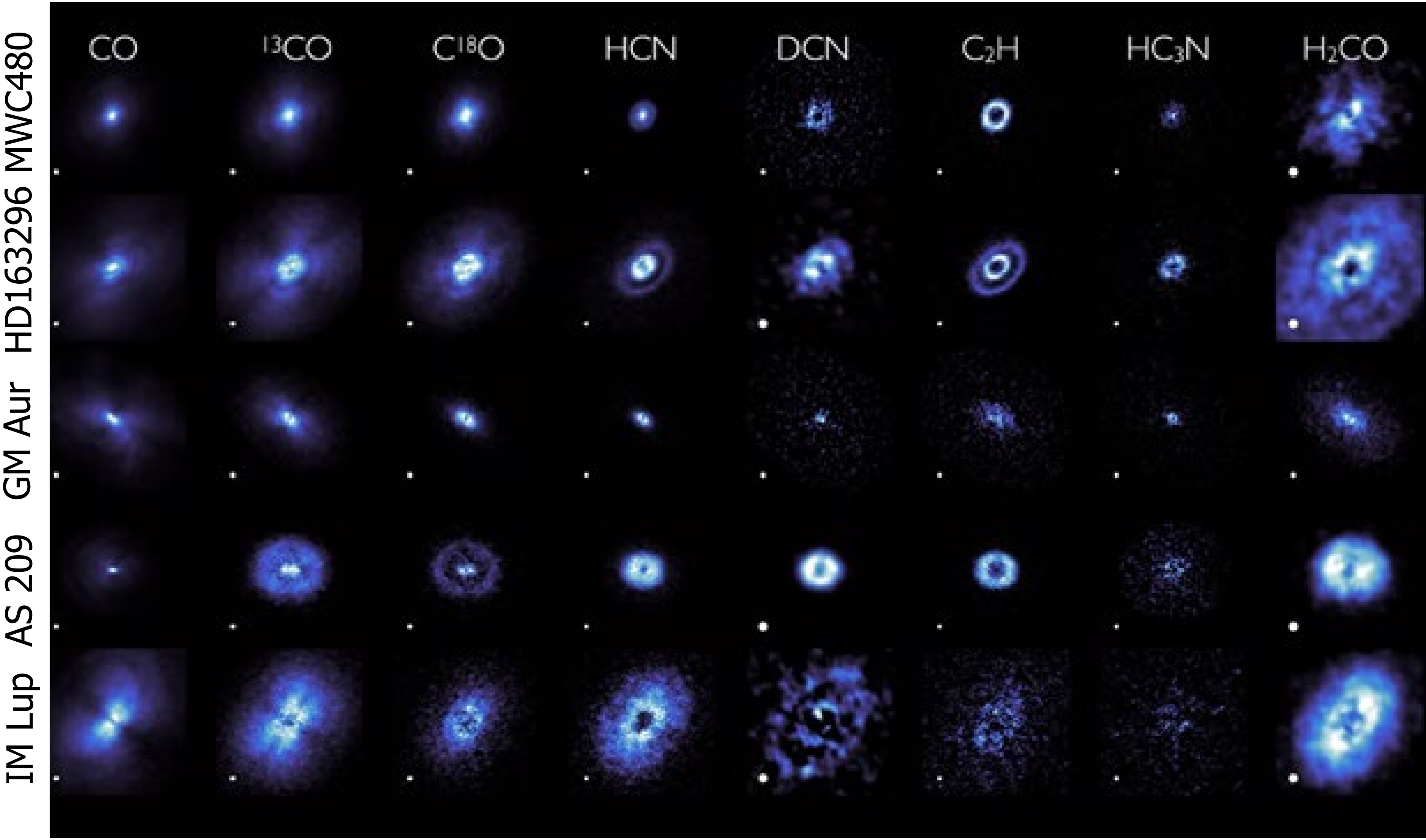
https://almascience.nao.ac.jp/almadata/lp/DSHARP/

Substructures (gasp, rings) exist universally in disks.

High Res. Obs. of Gas in Disks

https://almascience.eso.org/alma-data/lp/MAPS
http://alma-maps.info/

ALMA LP/MAPS (Oberg+ 2021)



Substructures (gasp, rings) are common in gas, too.

Obs. of Gas in Protoplanetary Disks

UV H_2 Lyman-Werner band transitions

Optical [OI] 6300A

NIR

H_2 v=1-0 S(1), S(0),
CO Δv=2, Δv=1,
H_2O, OH, HCN, C_2H_2, CH_4

MIR

H_2 v=0-0 S(1), S(2), S(4)

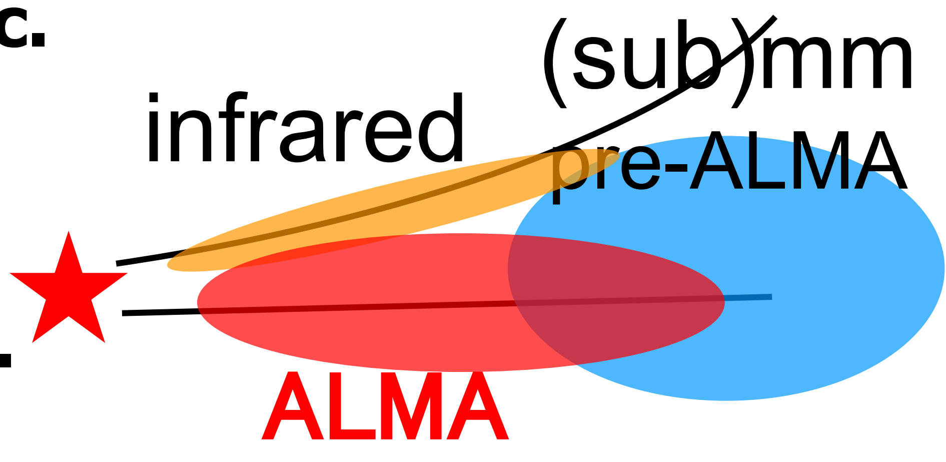
H_2O, OH, HCN, C_2H_2, CO_2, etc.
(Spitzer Space Telescope)

FIR

[OI] 63um, 145um,
CO, H_2O, CH^+, HD, NH_3, etc.
(Herschel Space Observatory)

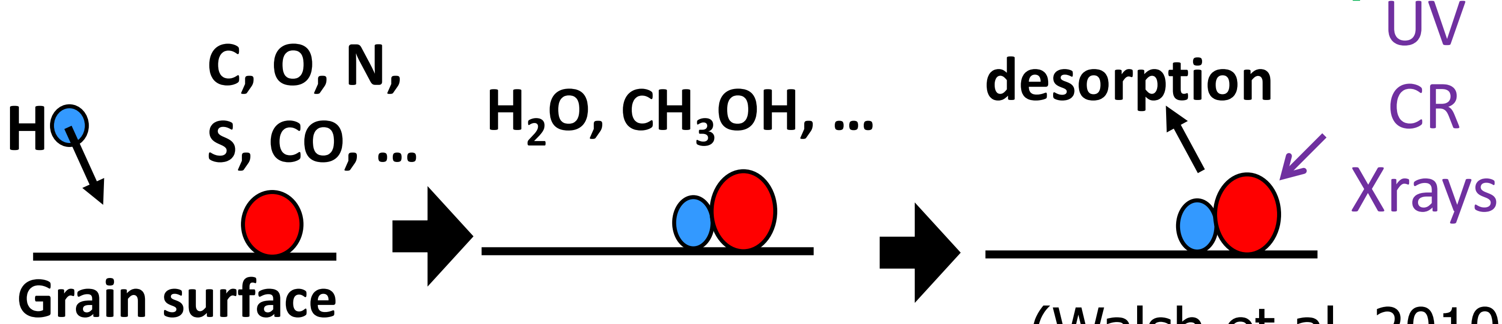
(sub)mm

CO, ^{13}CO, $C^{18}O$, $C^{17}O$, $^{13}C^{18}O$, $^{13}C^{17}O$, HCO^+, $H^{13}CO^+$, DCO^+, [CI], C_2H, C_2D, c-C_3H_2, H_2CO, HCOOH, CH_3OH, HCN, $H^{13}CN$, DCN, $HC^{15}N$, HNC, CN, $C^{15}N$, N_2H^+, N_2D^+, HC_3N, CH_3CN, CH_2CN, CS, $C^{34}S$, ^{13}CS, H_2S, SO, H_2CS, etc.

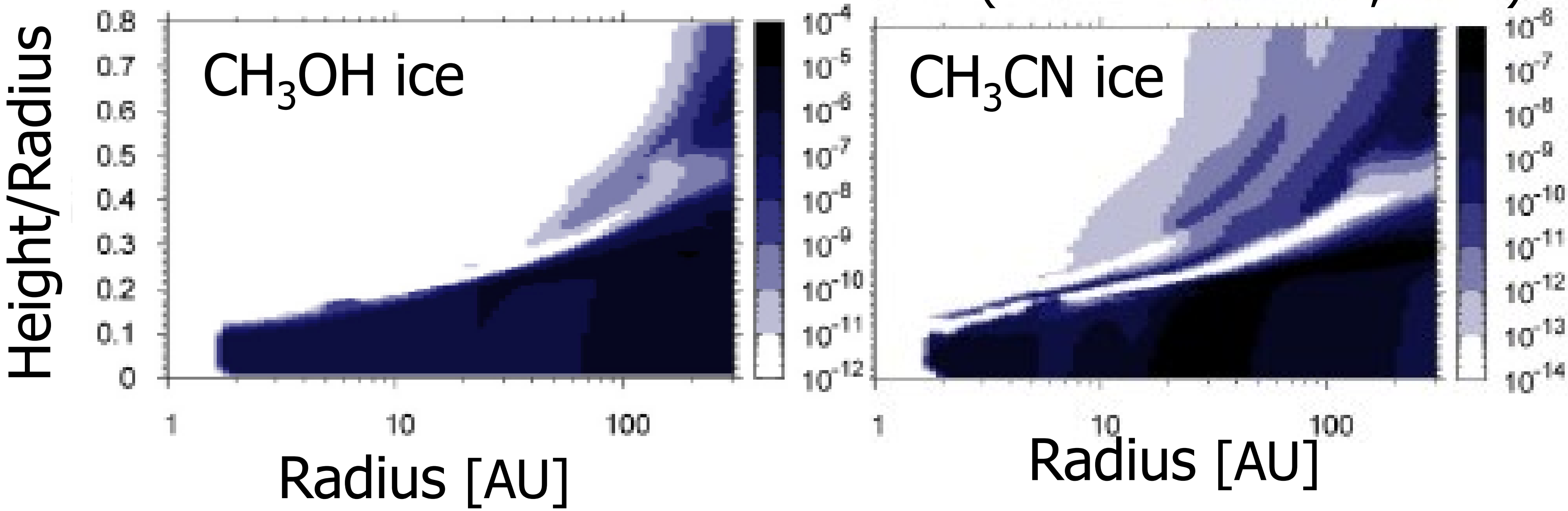


Modeling Complex Molecules in PPD

Grain surface reactions Photodesorption



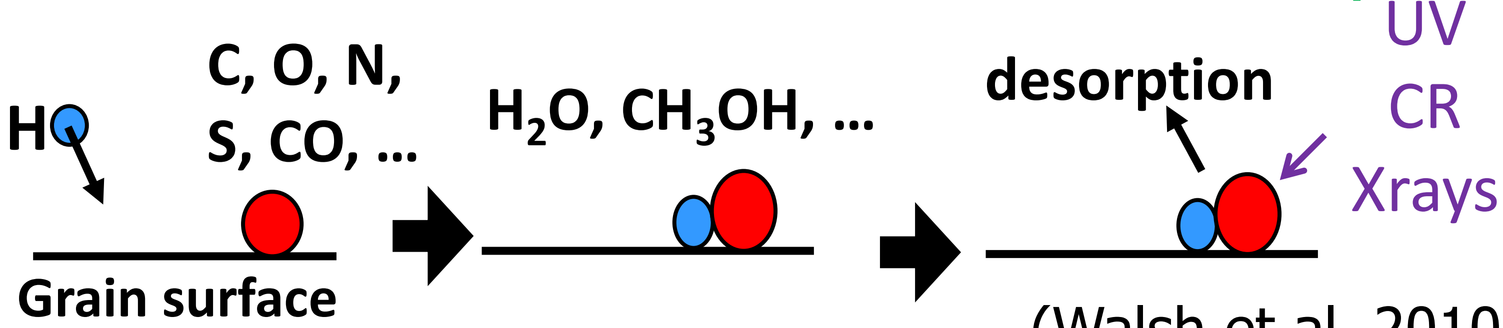
(Walsh et al. 2010, 2014)



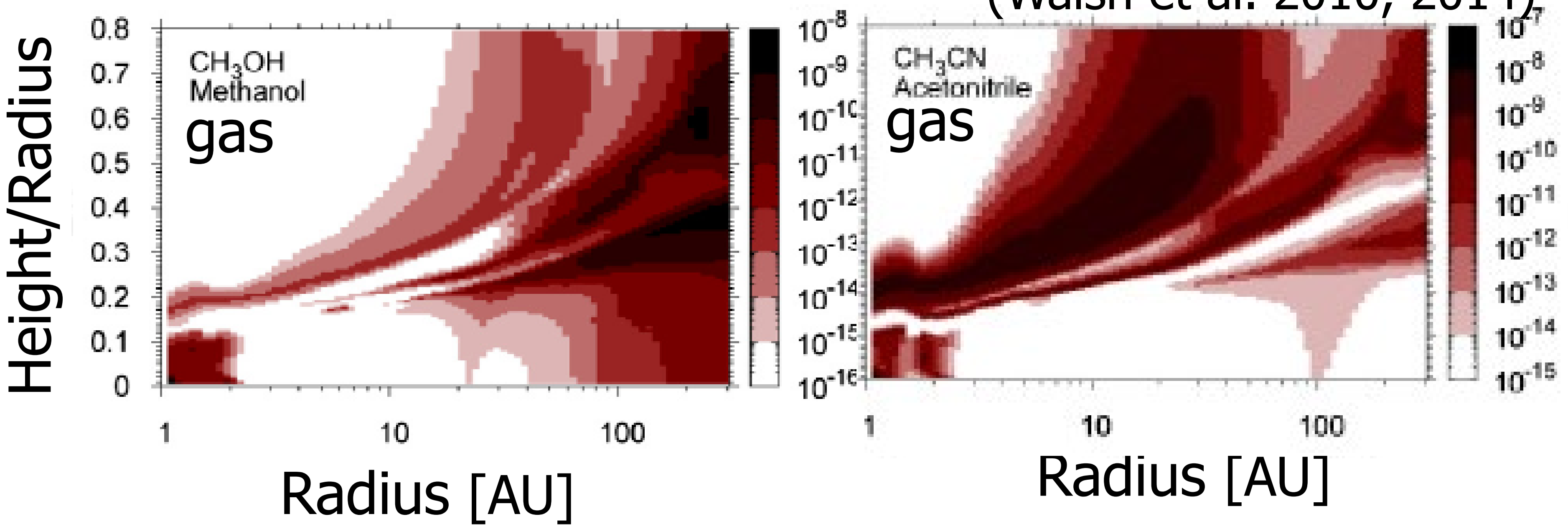
Complex organic mol. are formed efficiently by grain surface reactions near the disk midplane

Modeling Complex Molecules in PPD

Grain surface reactions   Photodesorption



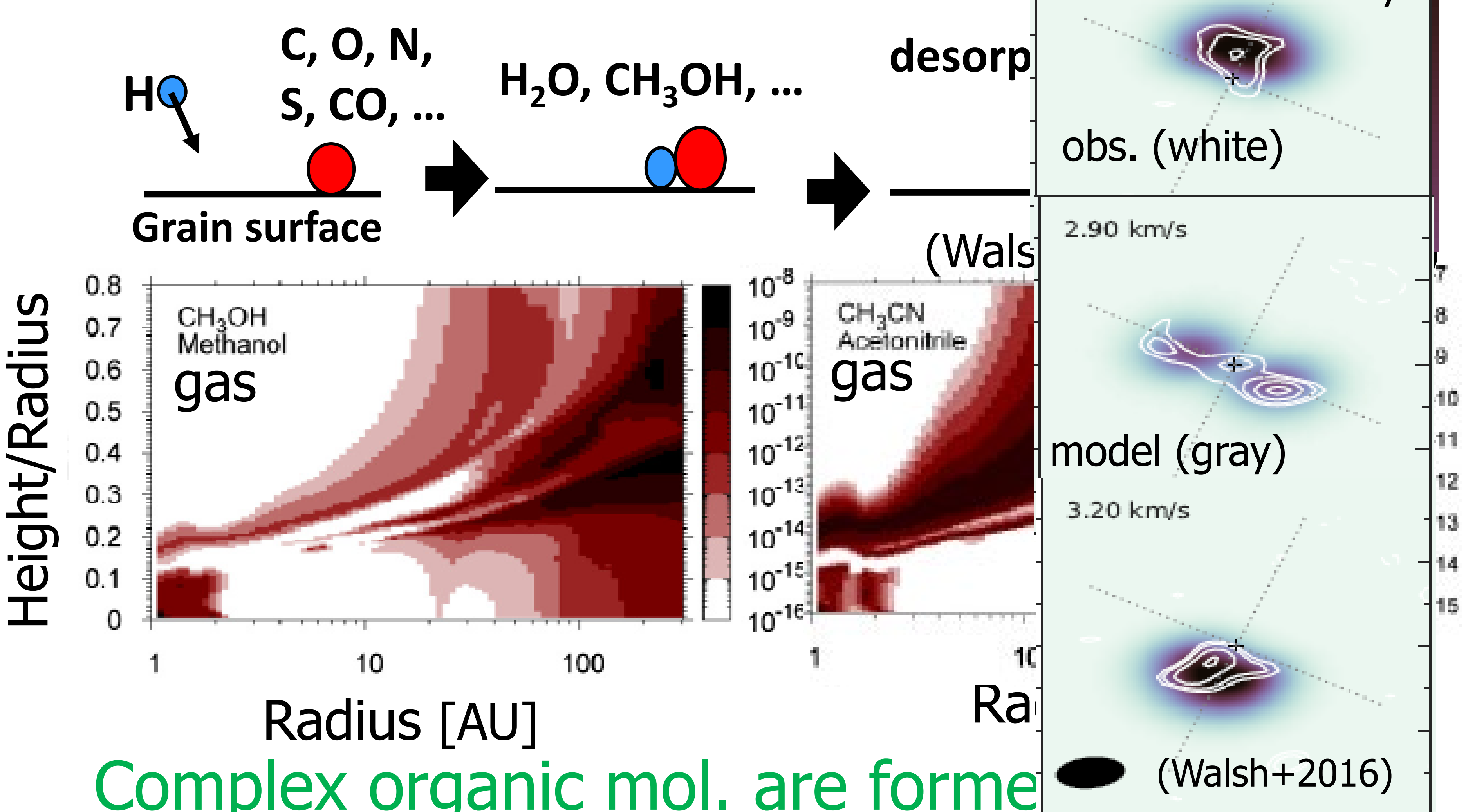
(Walsh et al. 2010, 2014)



Complex organic mol. are formed efficiently by grain surface reactions near the disk midplane

Modeling Complex Molecules in PPD

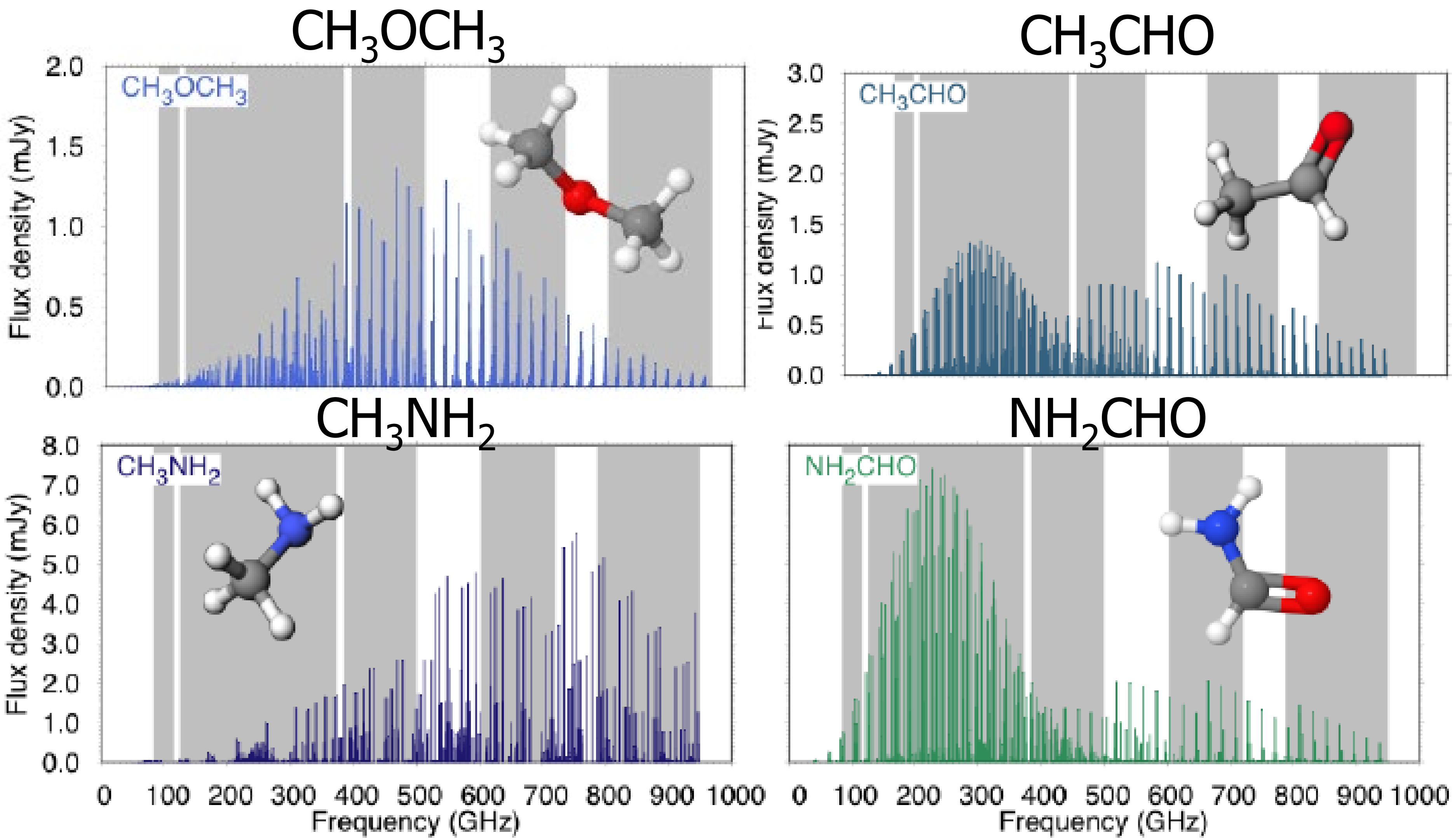
Grain surface reactions Photod



Complex organic mol. are forme

by grain surface reactions near the disk midplane

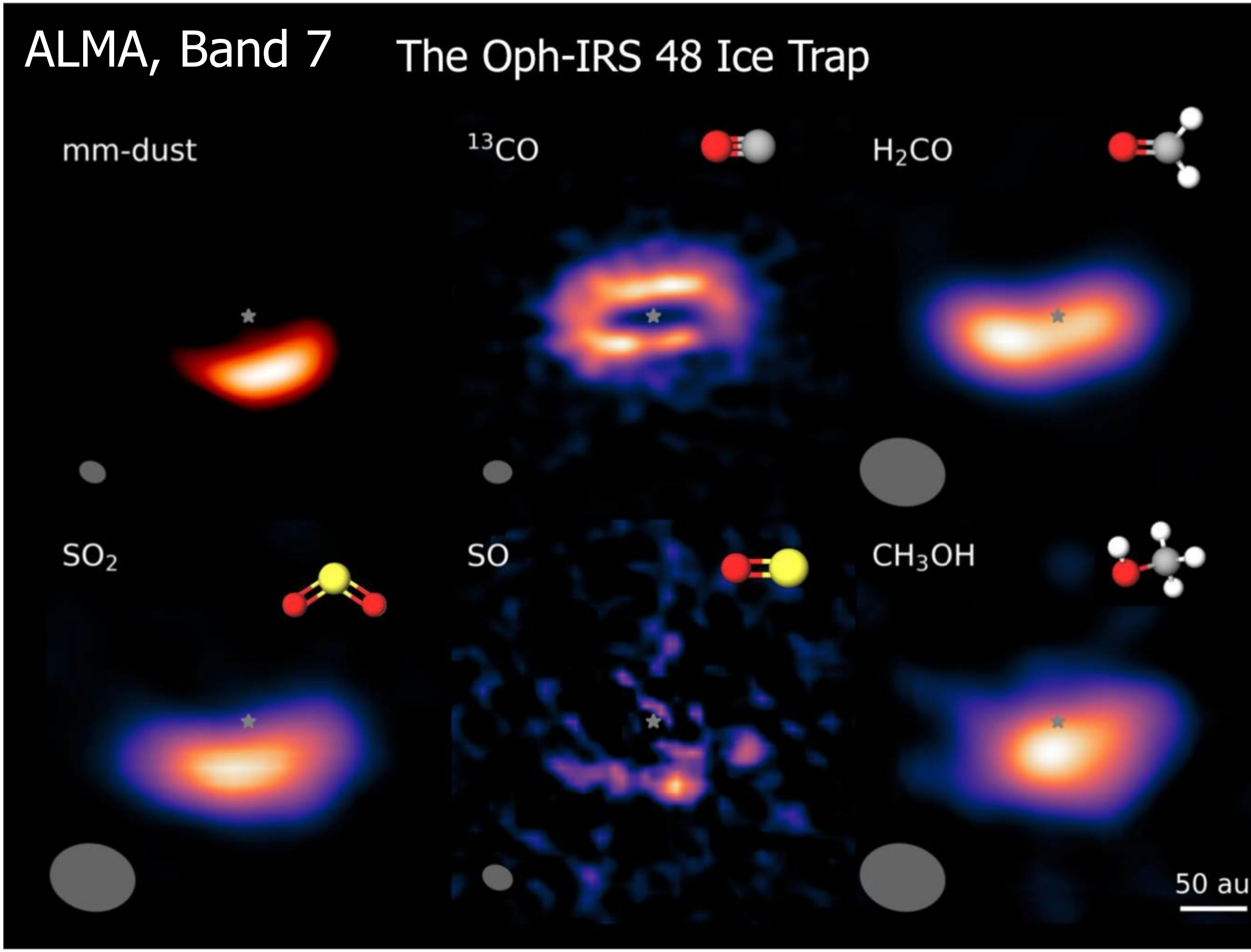
Model Spectra of More COMs in Disks



Searching more COMs in disks by ALMA & ngVLA!

(Walsh et al. 2017)

Broad Band Observations in Disks

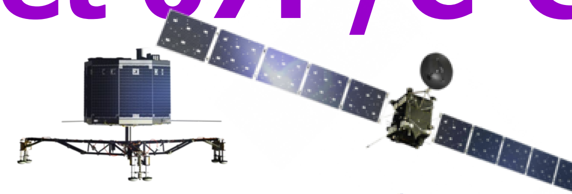


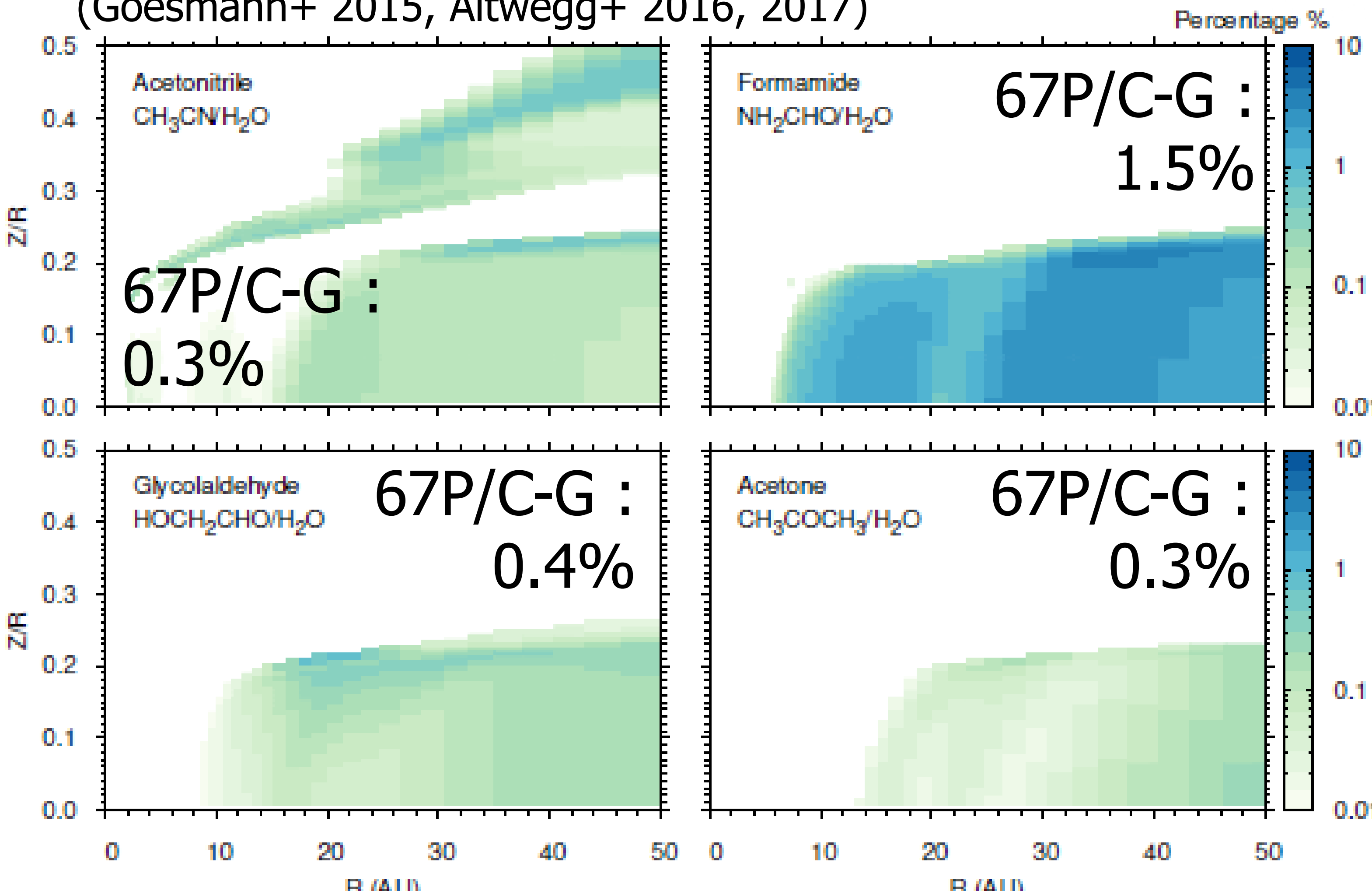
(van der Marel+2021, Booth+2021)

Further new discovery of molecules are reported.

COMs in Disks vs. Comet 67P/C-G

COMs in 67P/ Churyumov-Gerasimenko
COSAC/Philae, ROSINA, Rosetta
(Goesmann+ 2015, Altwegg+ 2016, 2017)



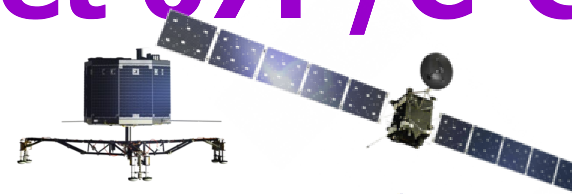


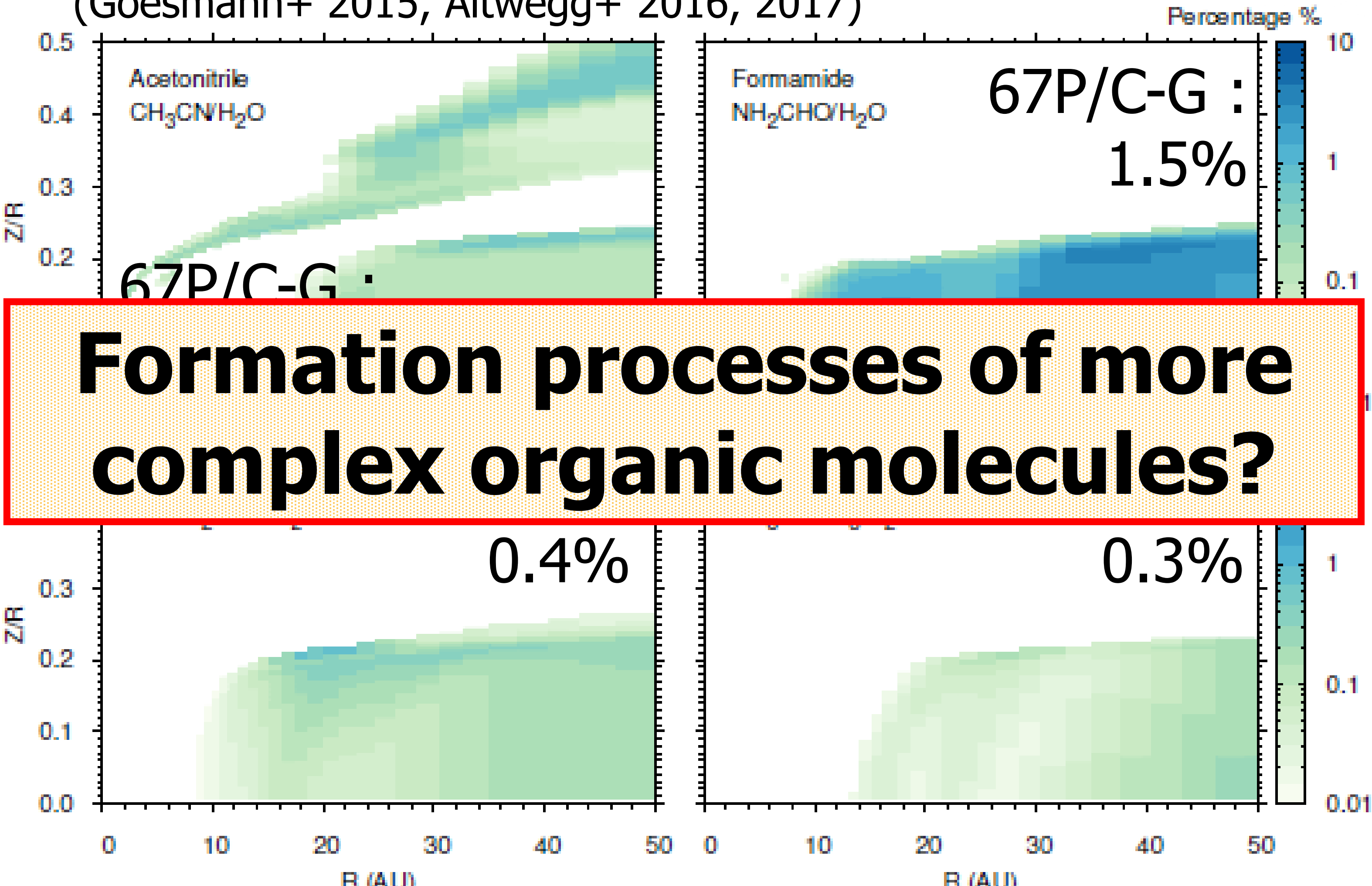
(Walsh et al. 2014, Walsh 2015)

Abundances of a part of molecules are consistent. More complete model is needed especially for larger molecules

COMs in Disks vs. Comet 67P/C-G

COMs in 67P/ Churyumov-Gerasimenko
COSAC/Philae, ROSINA, Rosetta
(Goesmann+ 2015, Altwegg+ 2016, 2017)



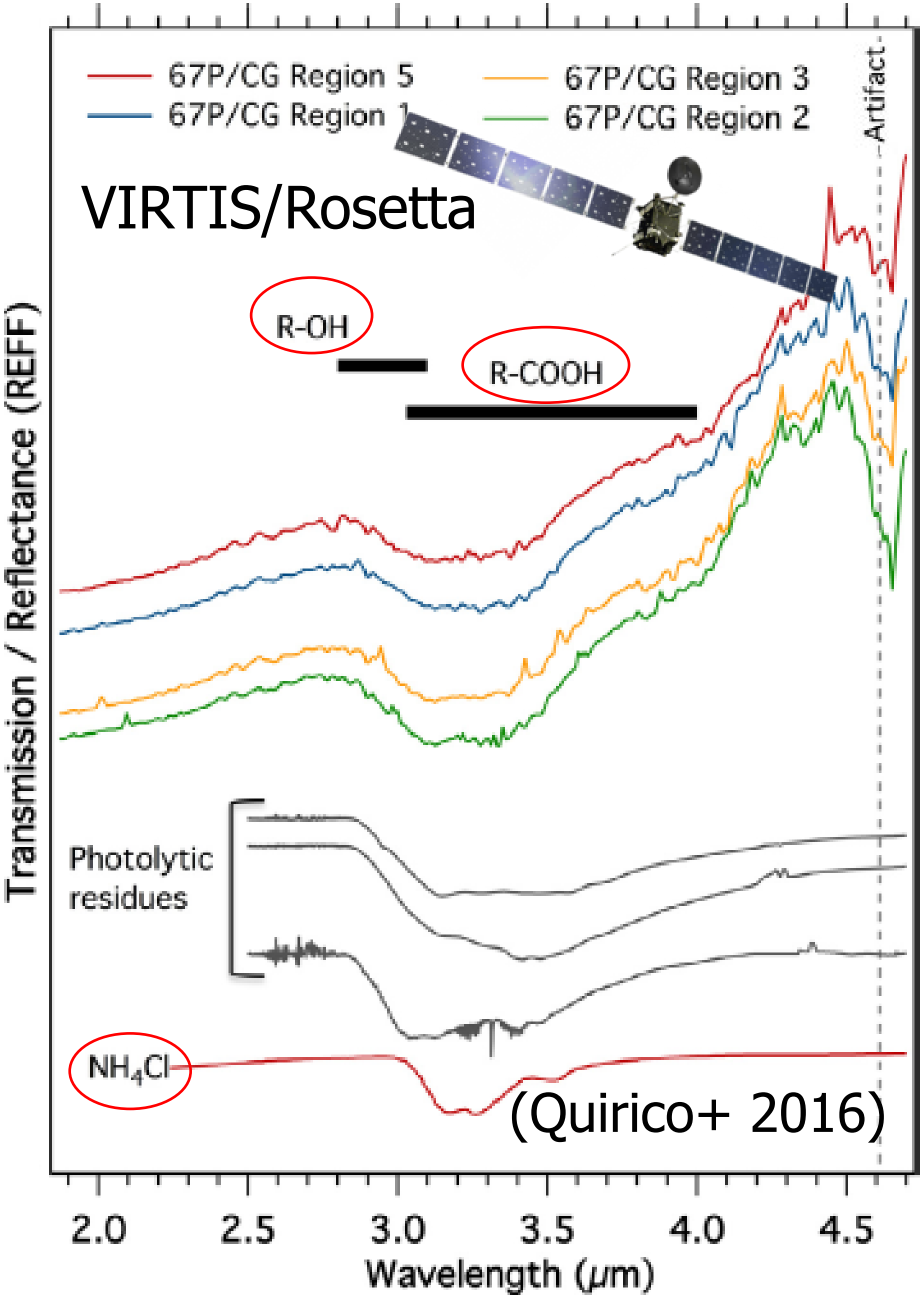


Formation processes of more complex organic molecules?

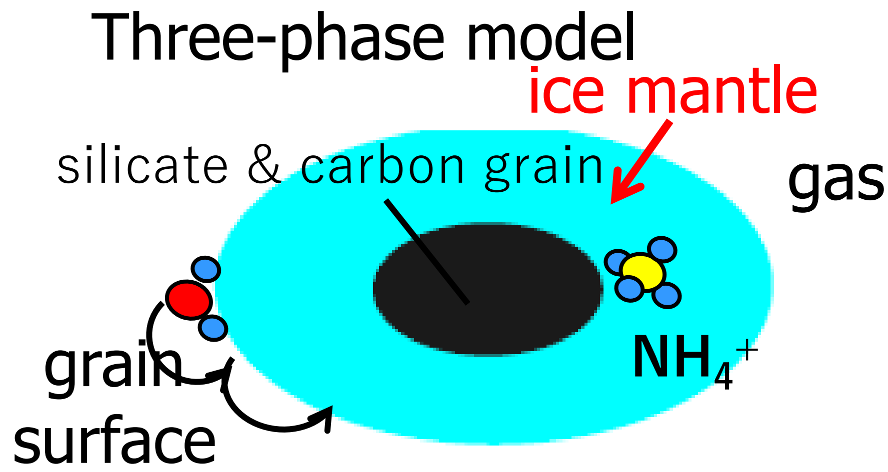
(Walsh et al. 2014, Walsh 2015)

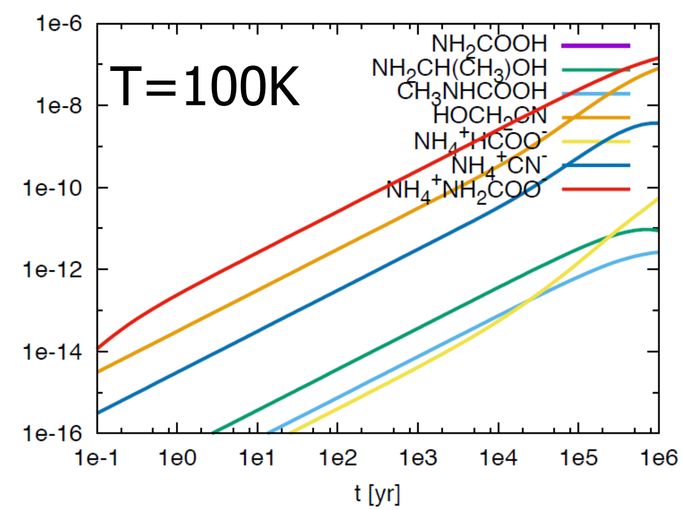
Abundances of a part of molecules are consistent. More complete model is needed especially for larger molecules

COMs in Disks vs. Comet 67P/C-G



New chemical modelling

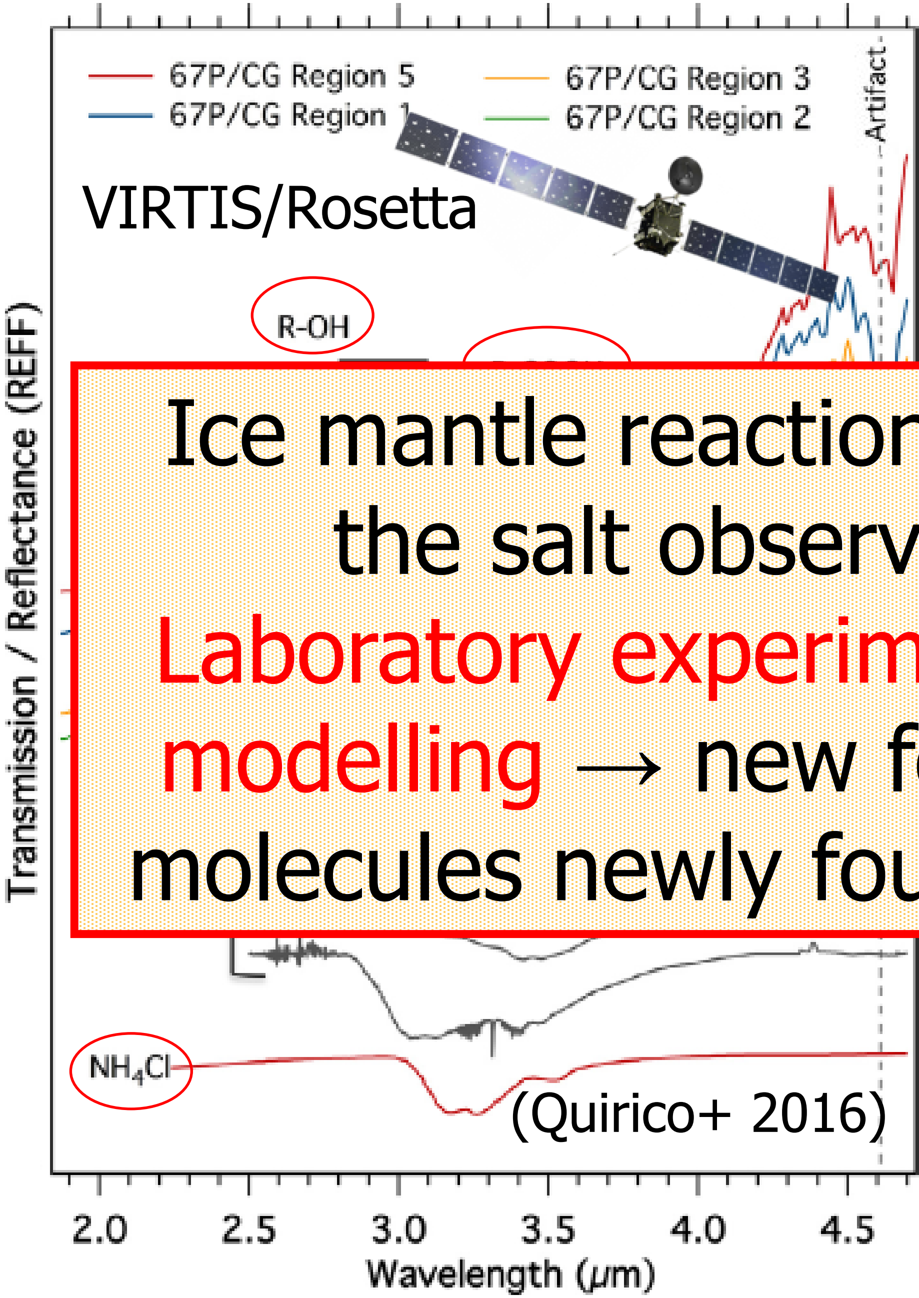




τ_{100K}=~10^6 year (Wei 2020)

→ Hayabusa 2, etc.

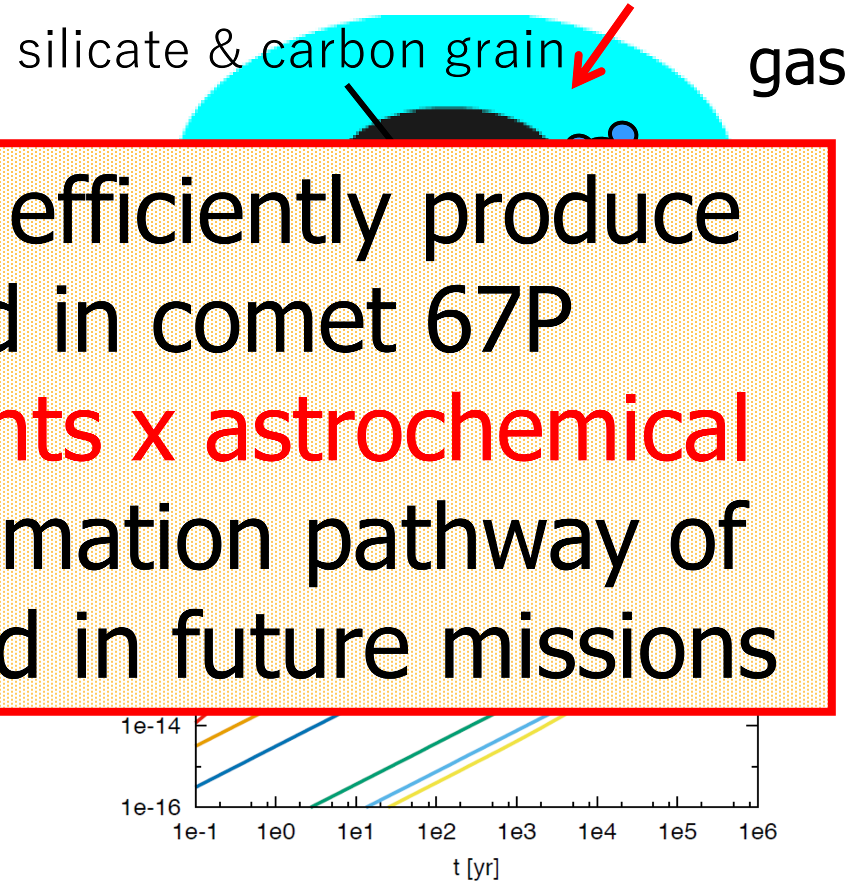
COMs in Disks vs. Comet 67P/C-G



(Quirico+ 2016)

New chemical modelling

Three-phase model



τ_100k=~10^6 year (Wei 2020)

→ Hayabusa 2, etc.

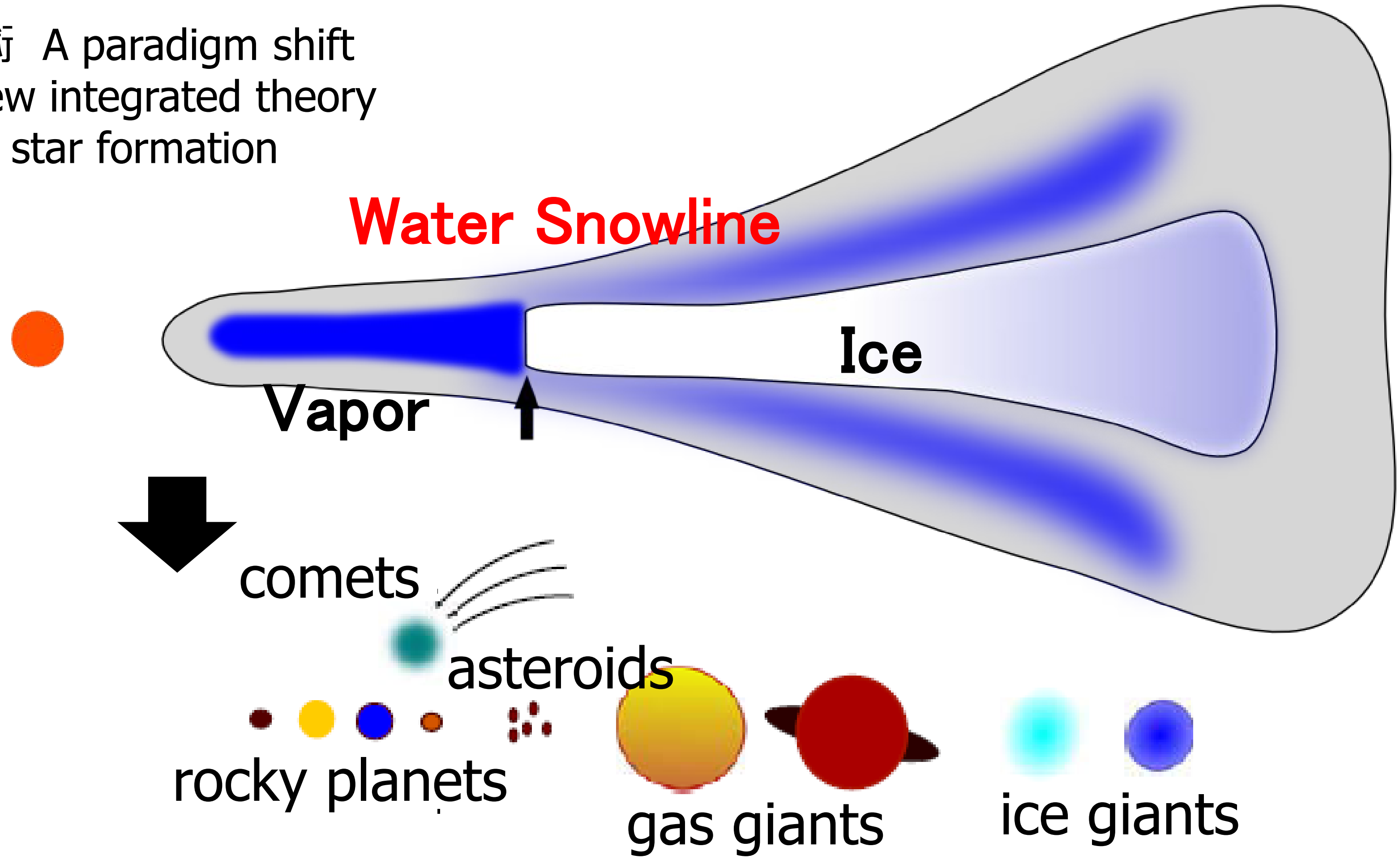
Ice mantle reactions efficiently produce the salt observed in comet 67P

Laboratory experiments x astrochemical modelling → new formation pathway of molecules newly found in future missions

Water Snowline in Planet Forming Disks

Boundary between Rocky & Gas Giant Planets

新学術　A paradigm shift
by a new integrated theory
of star formation



How do water snowline evolve during planet formation?
How do water and organics delivered to rocky planets?

Water Snowline in Planet Forming Disks

Boundary between Rocky & Gas Giant Planets

新学術　A paradigm shift
by a new integrated theory
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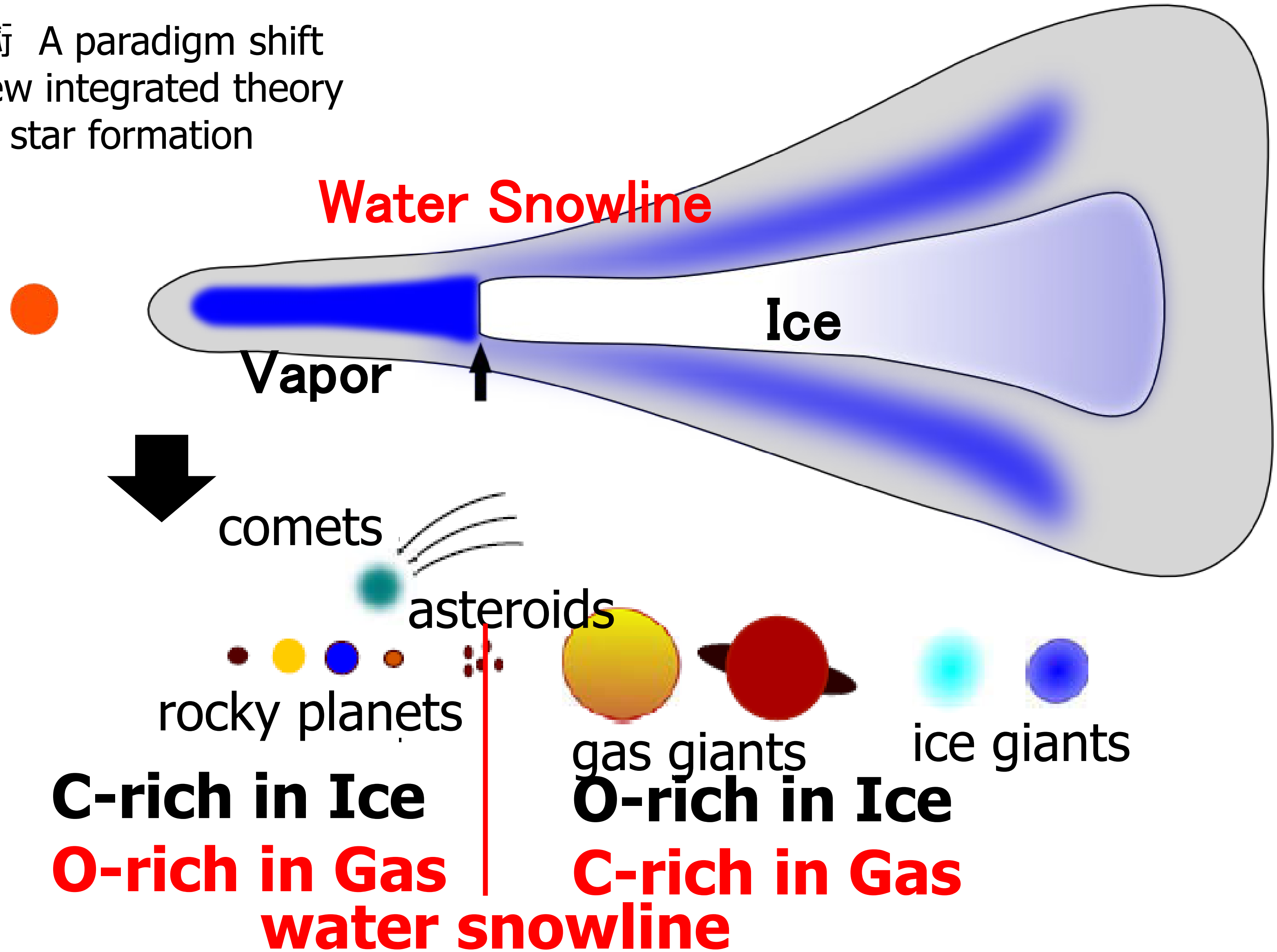
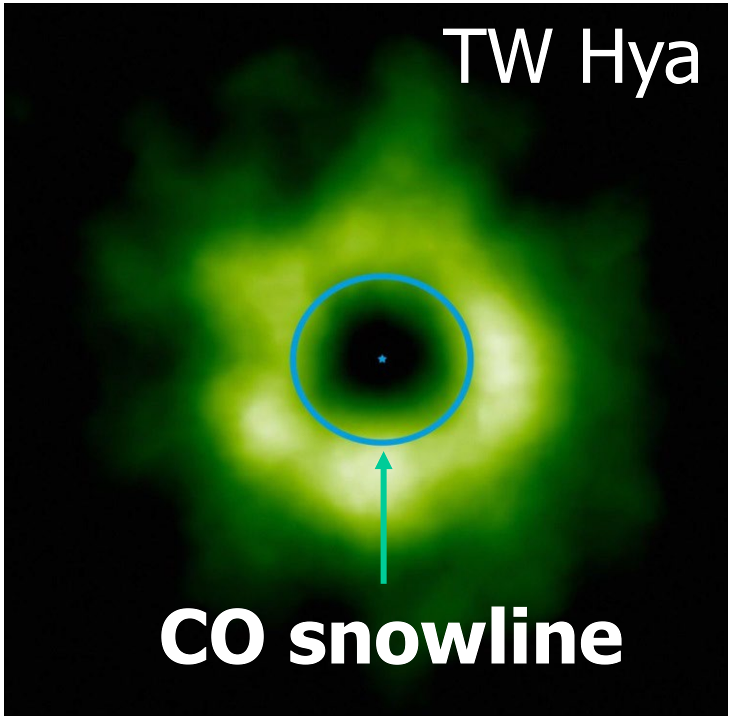
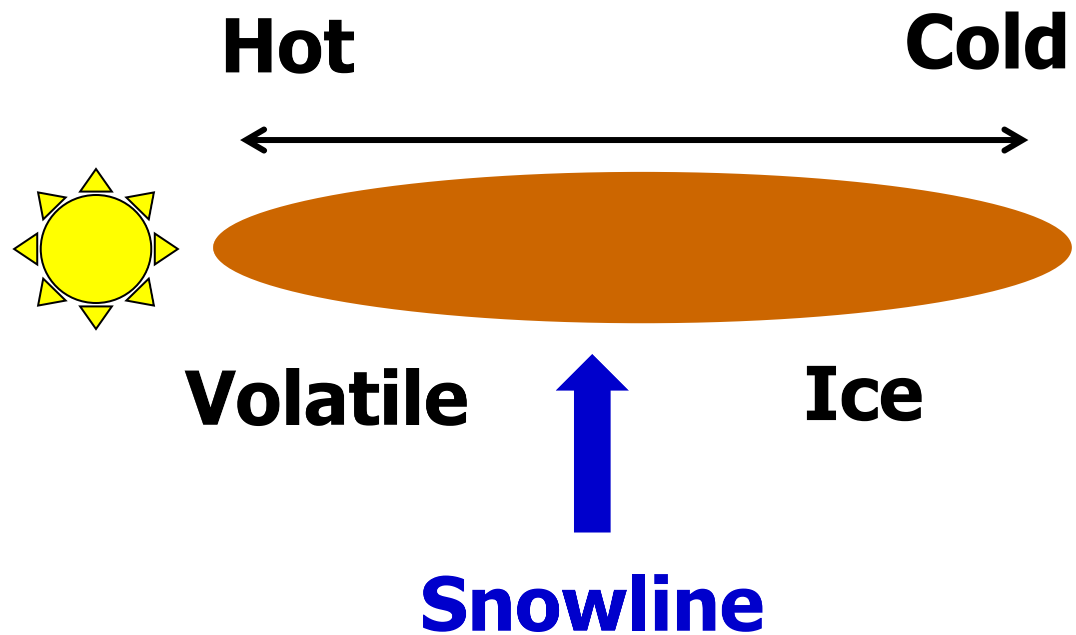


ALMA Observations of CO Snowline

(Qi et al. 2013)

N_2H^+ gas image



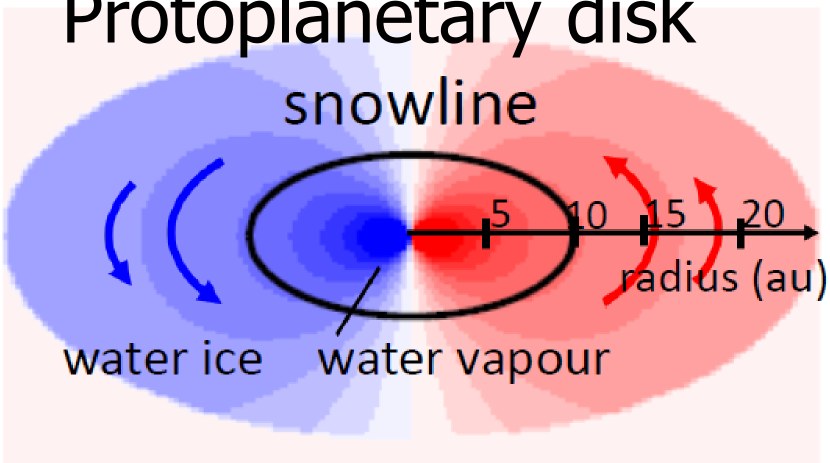


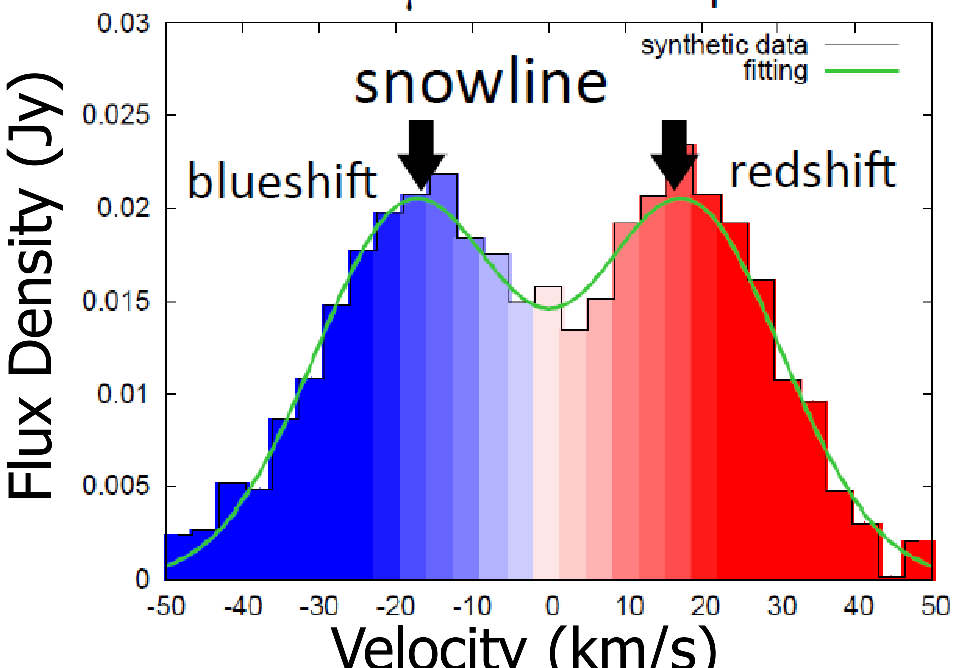
N_2H^+ gas distribution traces CO snowline.
(N_2H^+ is destroyed by CO in gas-phase.)

Observations of water snowline?

How to Observe Water Snowline?

GREX-PLUS survey





Keplerian rotation

$$\Delta v = \sqrt{\frac{GM_s}{r}} \sin i$$

i: inclination

Water snowline can be located by observing Doppler-shift of Keplerian rotation

Suitable line @ 17.75 μm

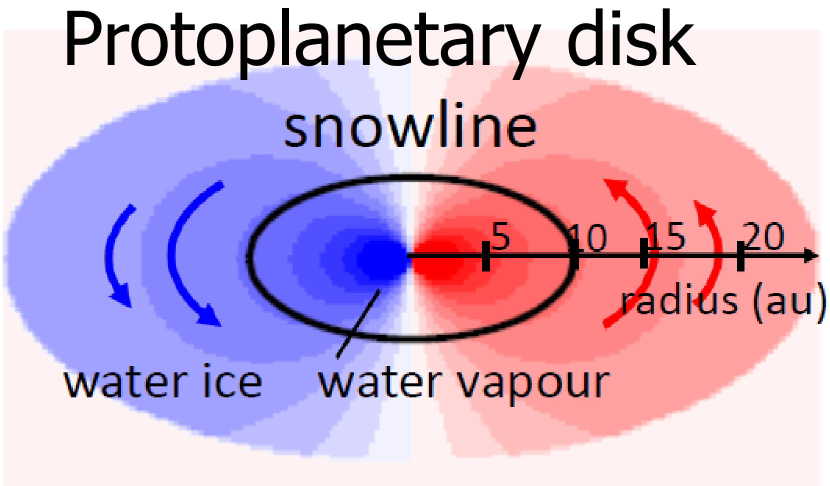
Typical line width of water from PPDs ~ 30km/s

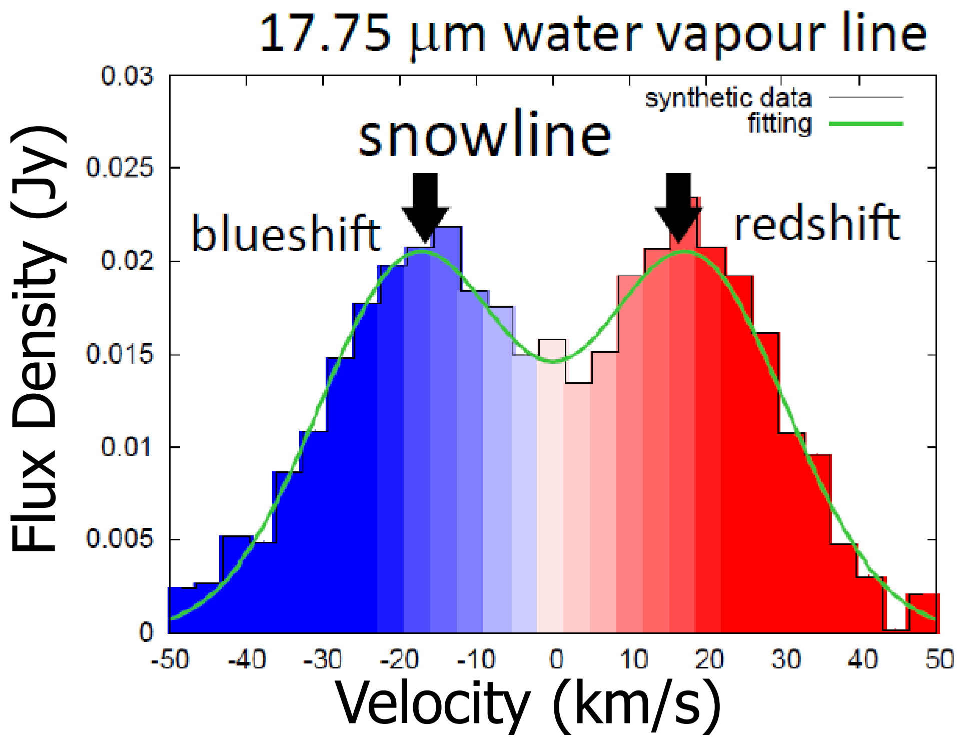
→ high-R (R ~ 30,000) is required to locate snowline

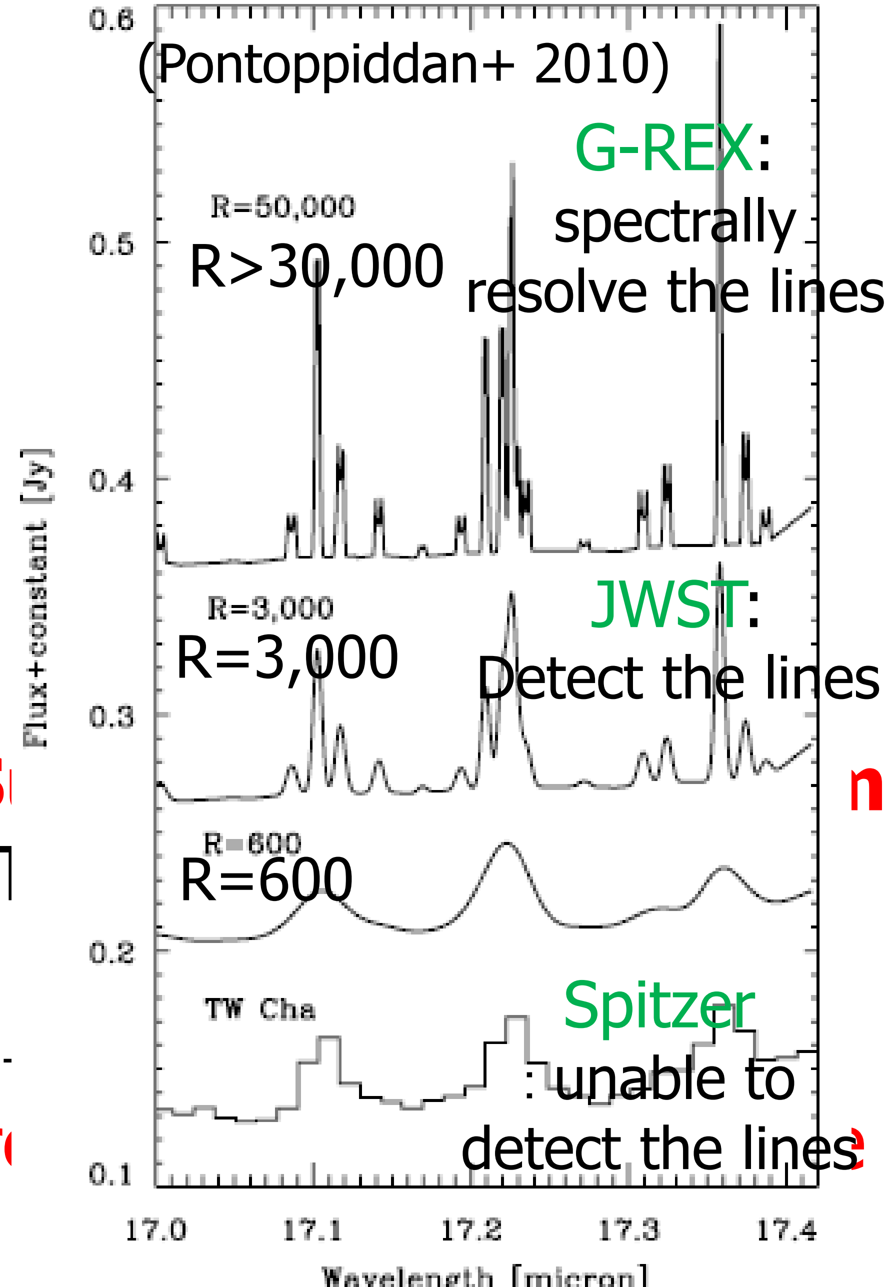
(Notsu+ 2016, 2017, Kamp+2021)

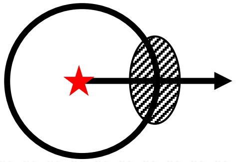
How to Observe Water Snowline?

GREX-PLUS survey



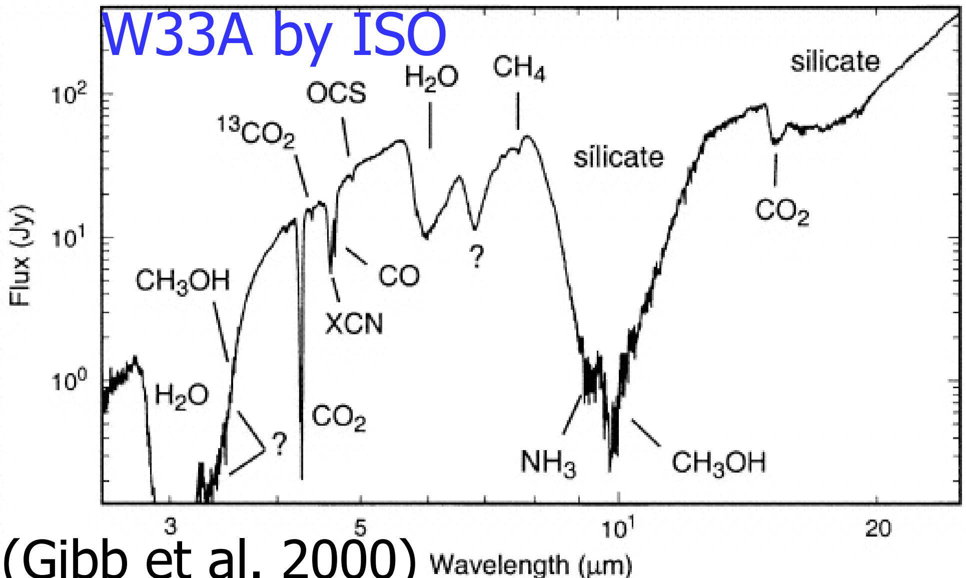






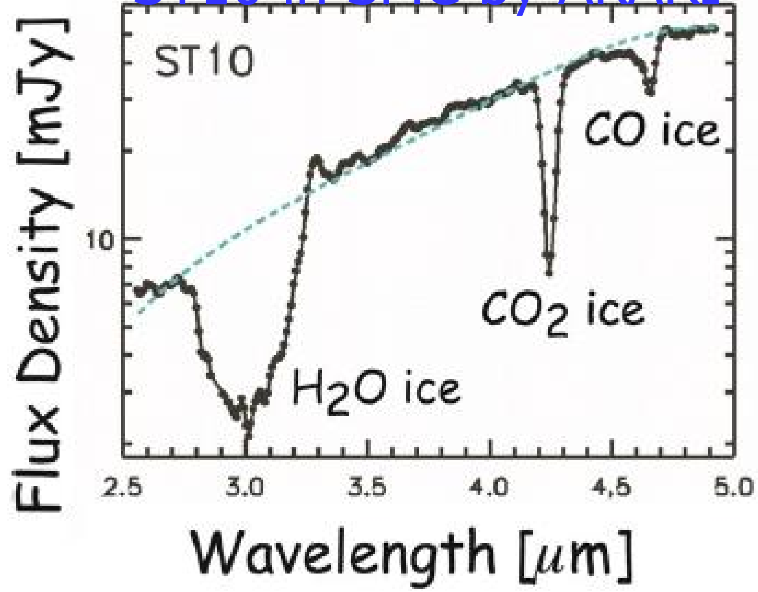
Molecules in Interstellar Ice

W33A by ISO



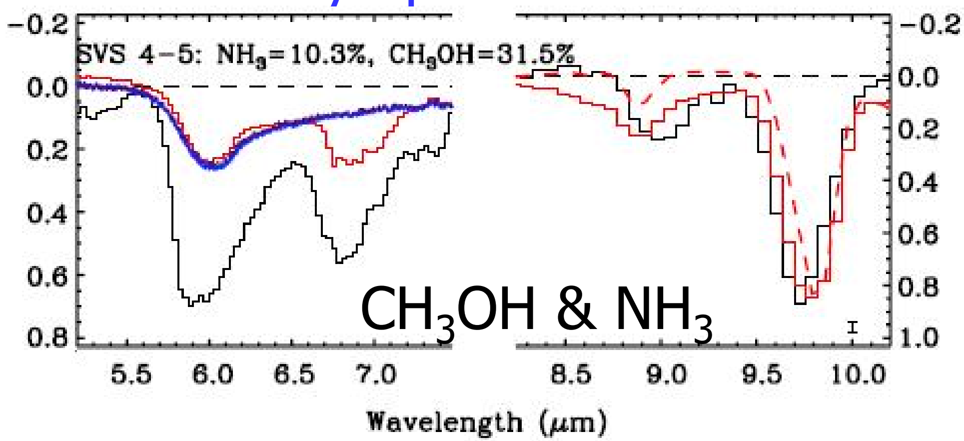
(Gibb et al. 2000)

ST10 in SMC by AKARI



(Shimonishi et al. 2010)

SVS 4-5 by Spitzer



CH_3OH & NH_3

(Bottinelli et al. 2010)

Si, C H_2O, CO, CH_3OH, ...

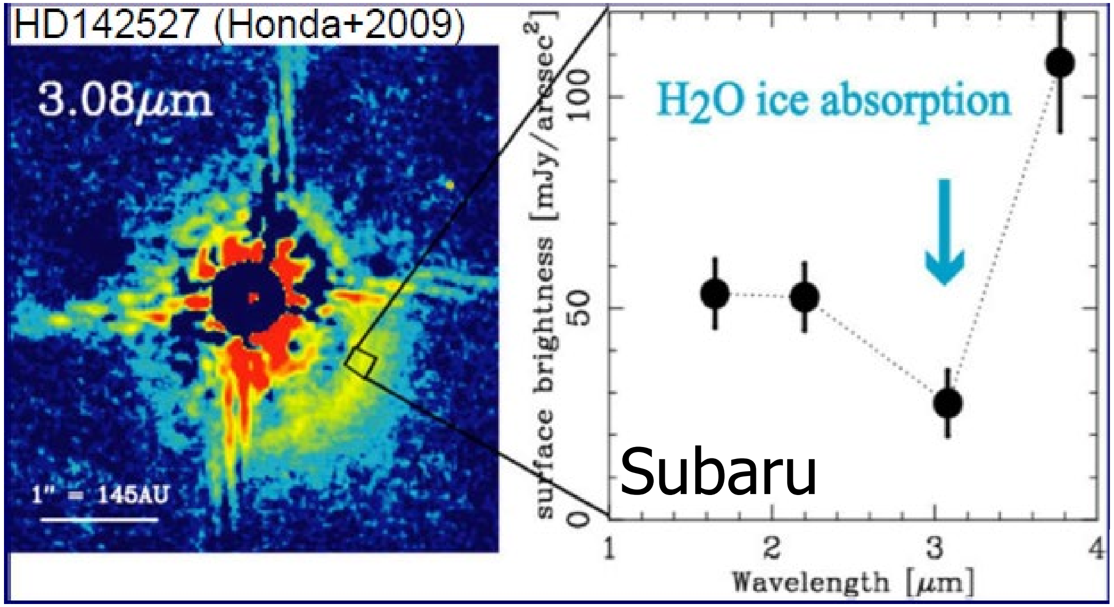
Observations of ice components by infrared spectroscopy

→ JWST, TMT, ..

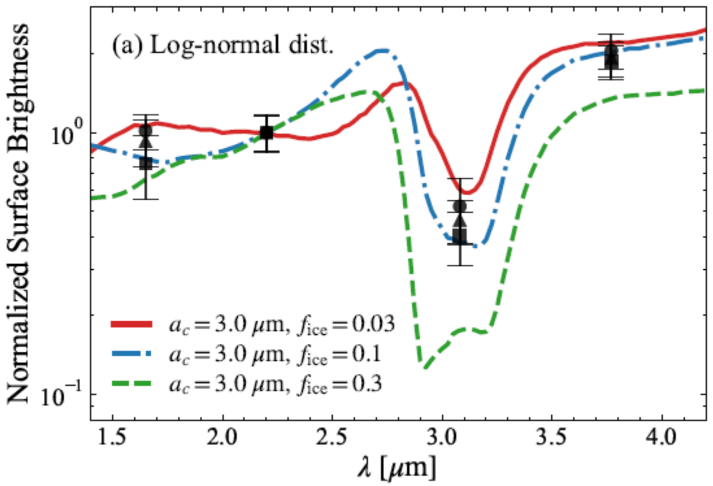
(e.g., Spitzer: Boogert+ 2008, Pontpiddan+ 2008, Oberg+ 2008, AKARI: Aikawa+2009, ..)

How to Observe Water Snowline?

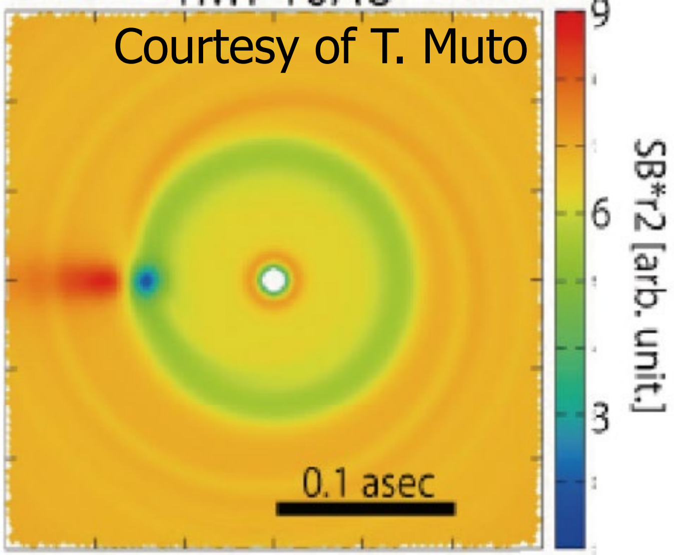
Water ice absorption in scattered light



(Tazaki+2021)



TMT 10AU

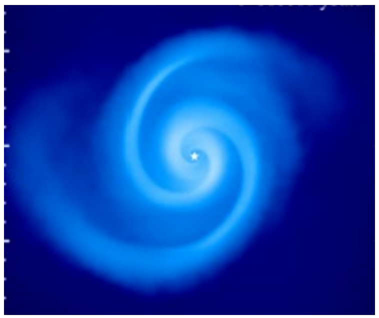


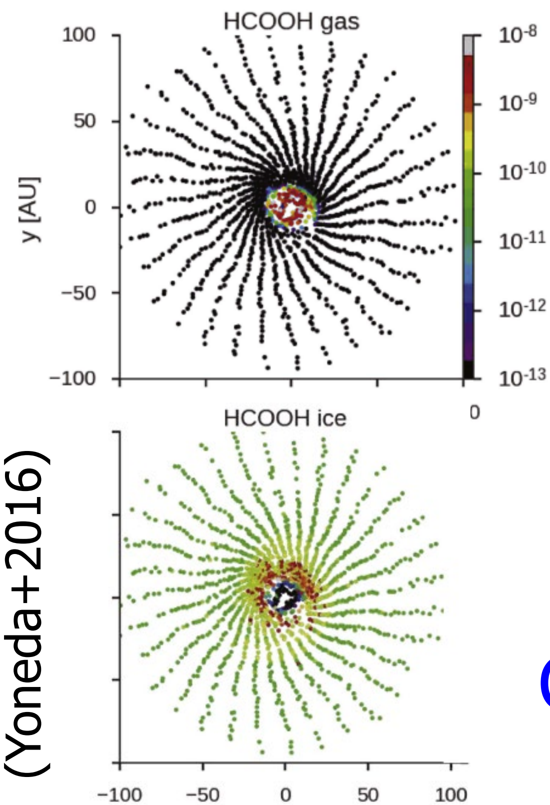
(Subaru2/TMT science)

TMT with smaller IWA will be able to trace water snowline in scattered light imaging observations

Chemistry with Dynamical Process?

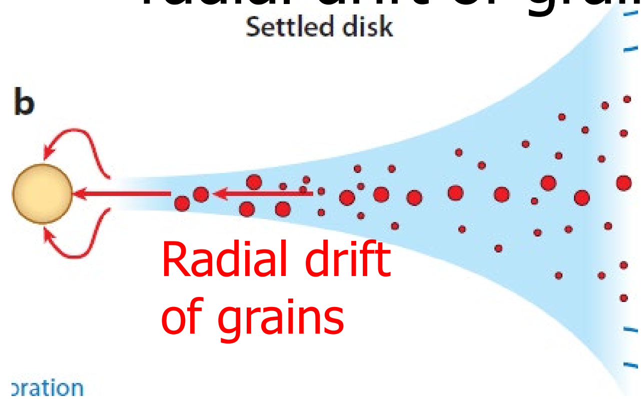
Chemistry in dynamical accretion phase



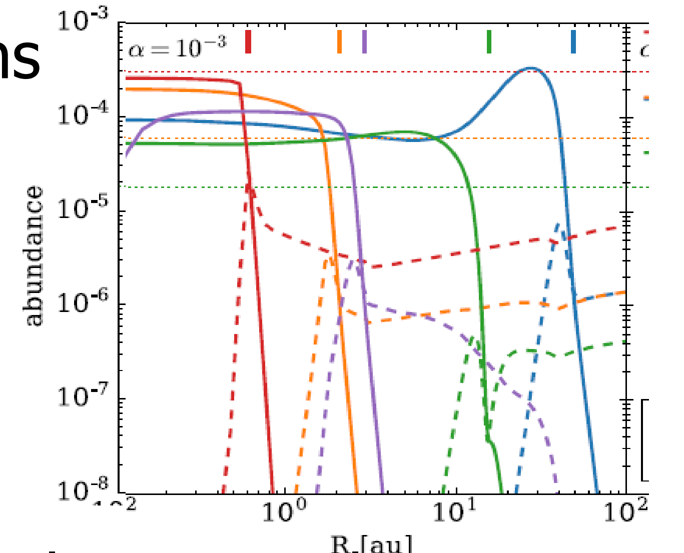


(Yoneda+2016)

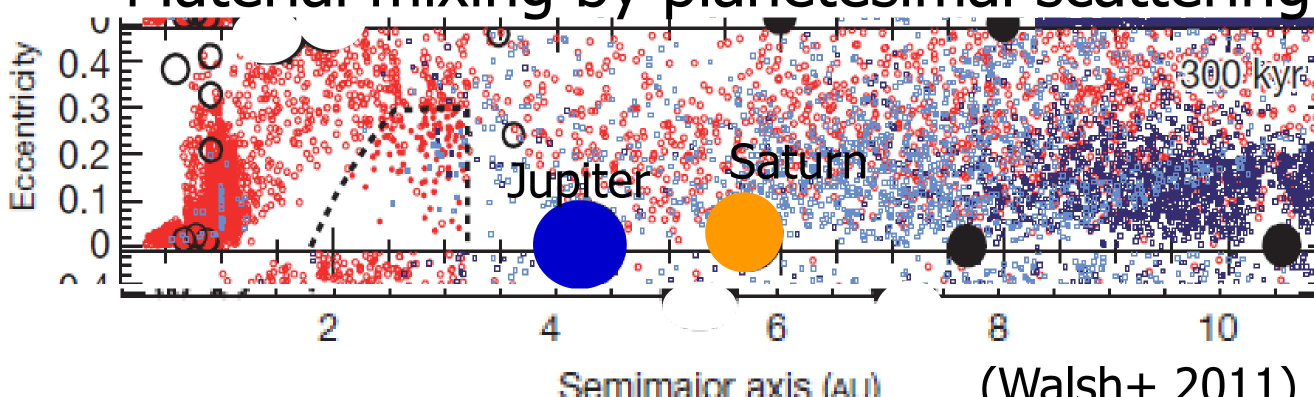
Chemistry along radial drift of grains



(Booth & Ilee 2019)



Material mixing by planetesimal scattering



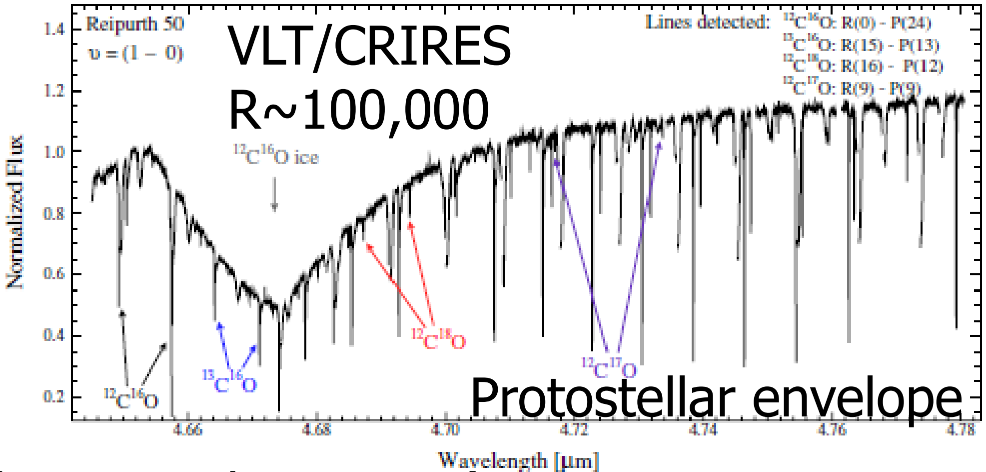
(Walsh+ 2011)

→ high performance computers

Chemical evolution should be considered together with dynamical processes

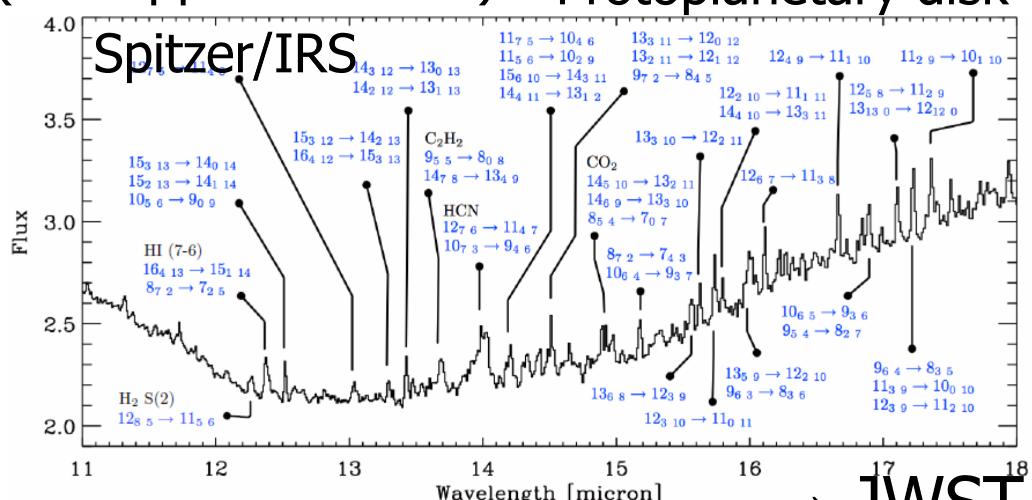
Infrared Spectroscopy for Material Evolution

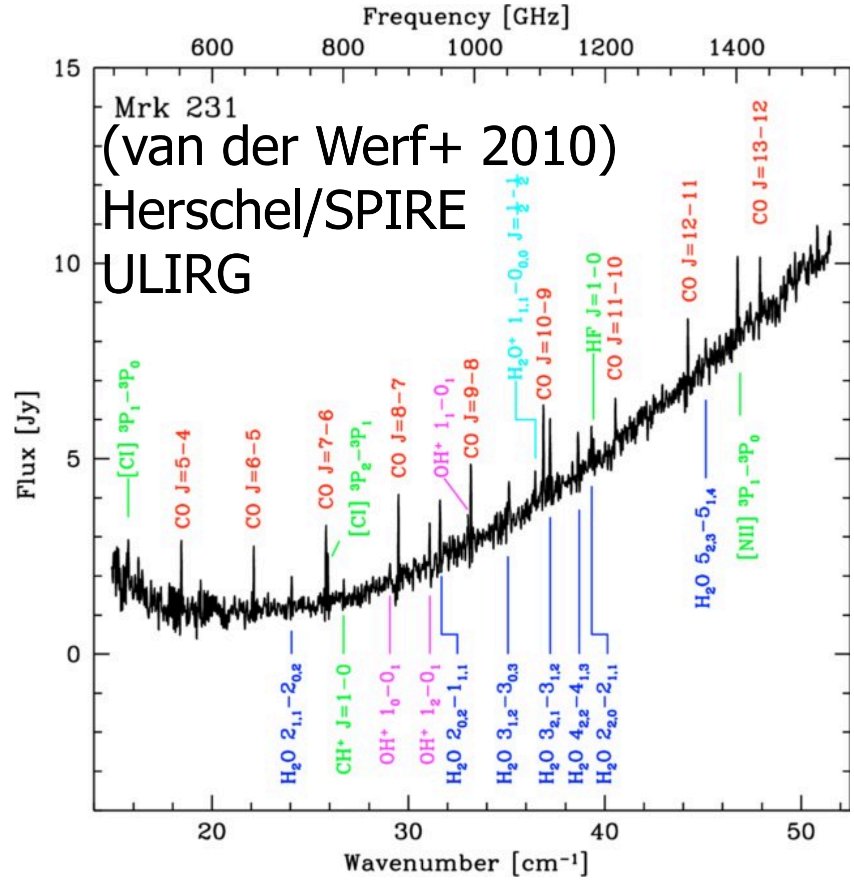
(Smith, Pontoppidan+ 2009)



(Pontoppidan+ 2010)

Protoplanetary disk

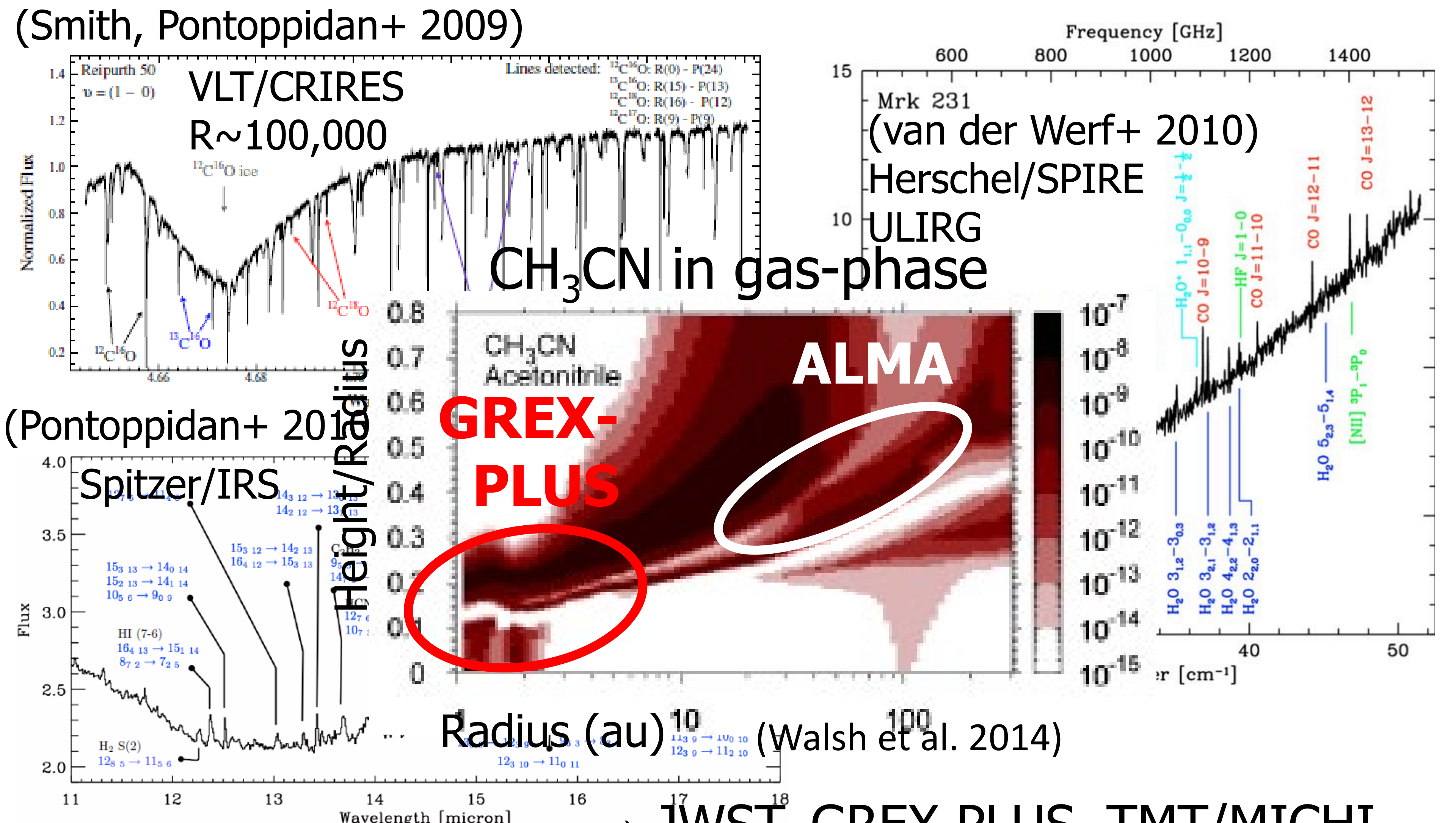




→ JWST, GREX-PLUS, TMT/MICHI, ..

Infrared spectroscopy will reveal molecular composition of gas & ice in various environments

Infrared Spectroscopy for Material Evolution



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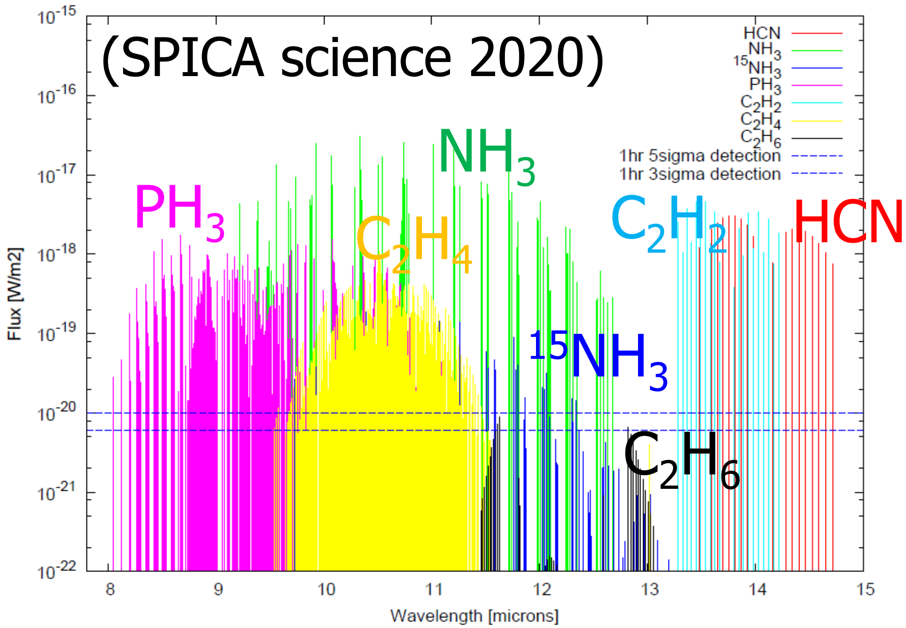
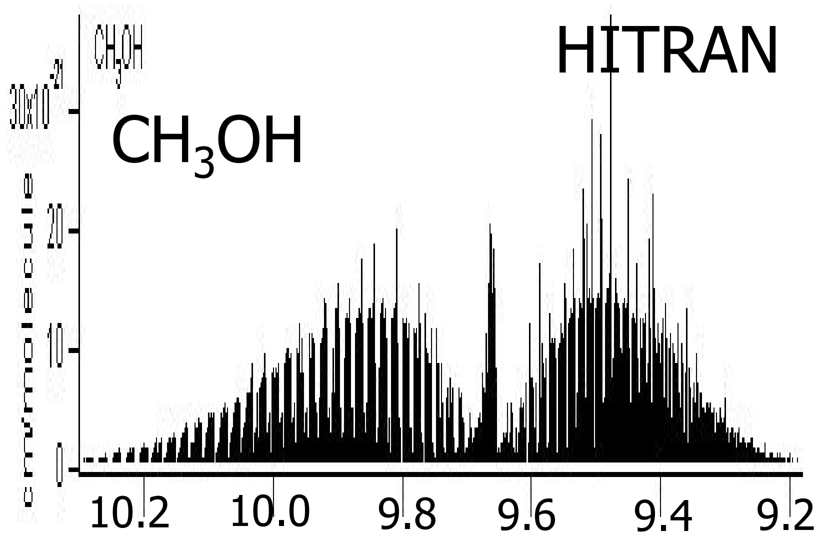
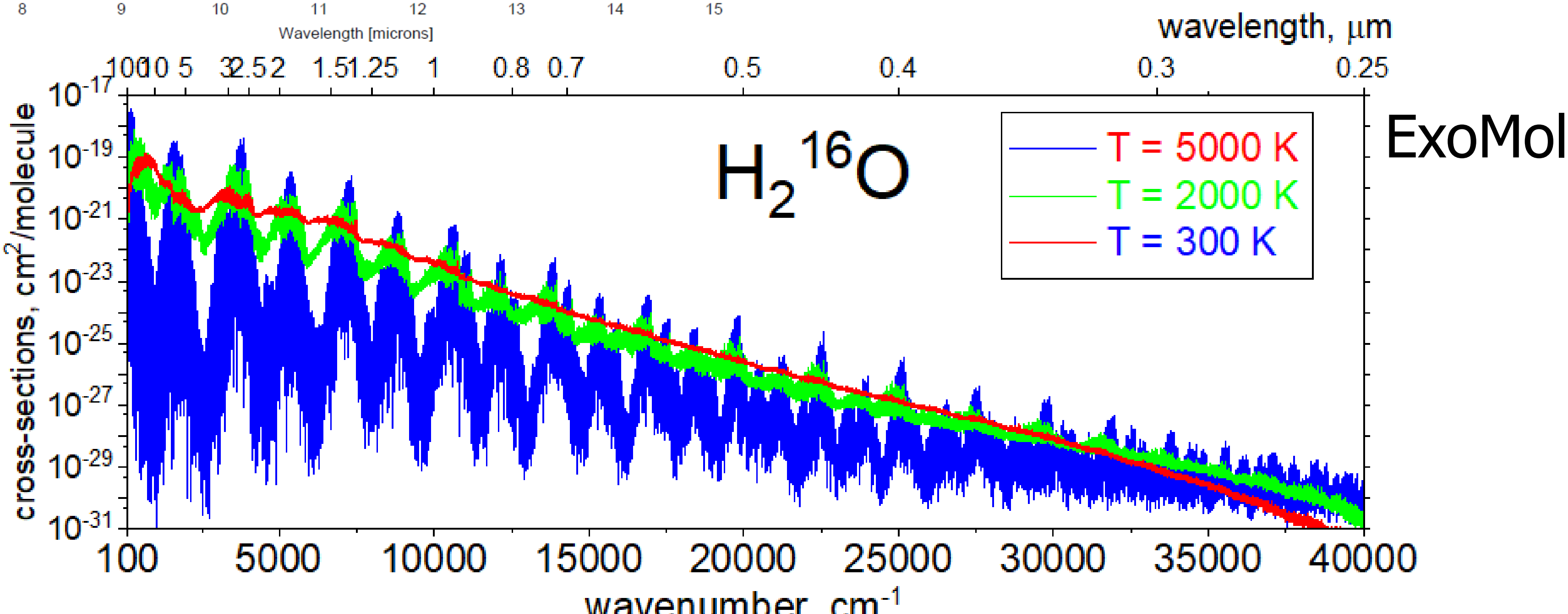
Infrared Spectroscopy for Material Evolution





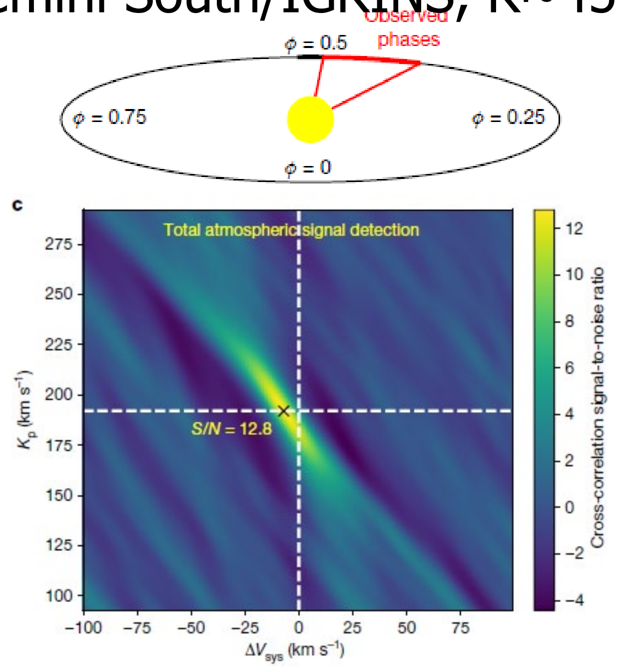


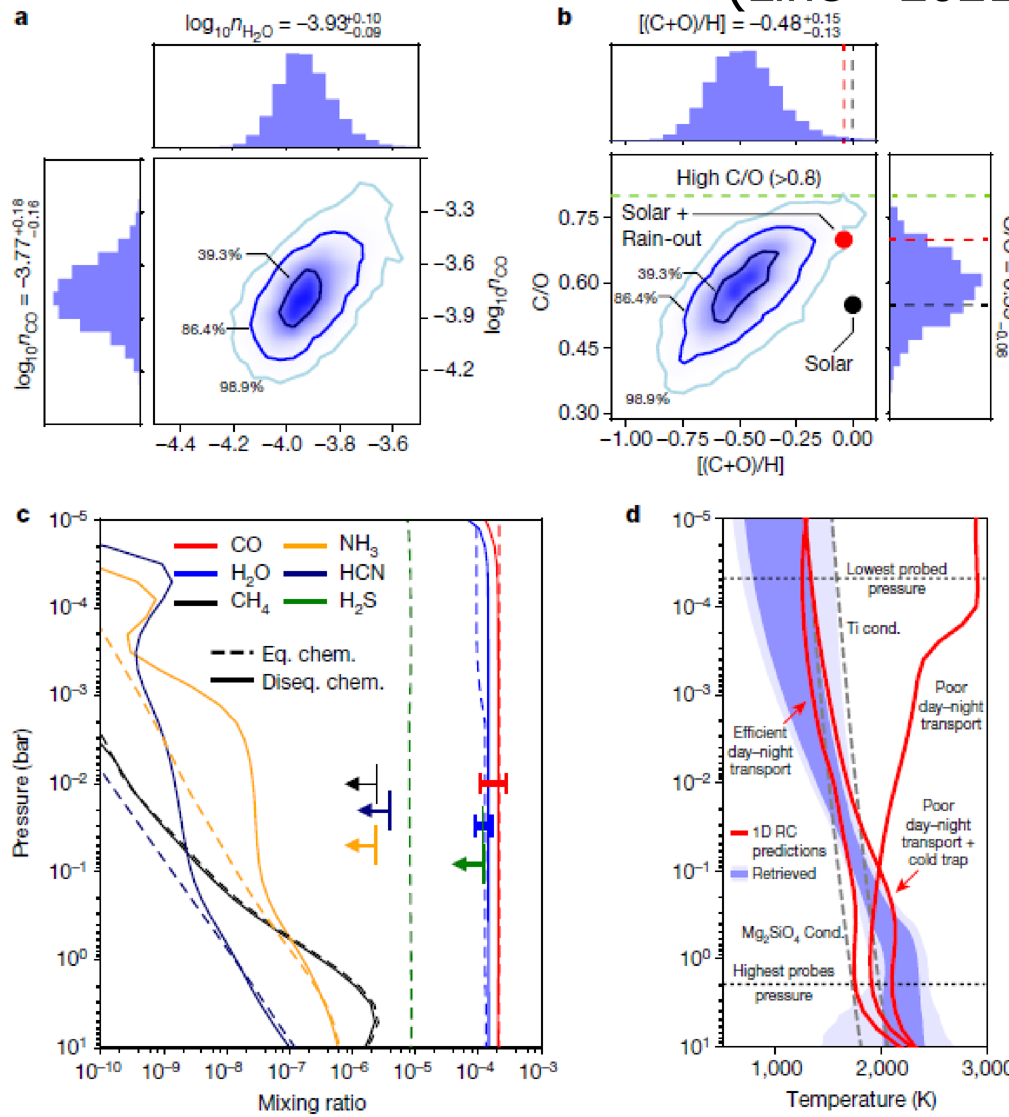
Collaborations with spectroscopists are necessary.

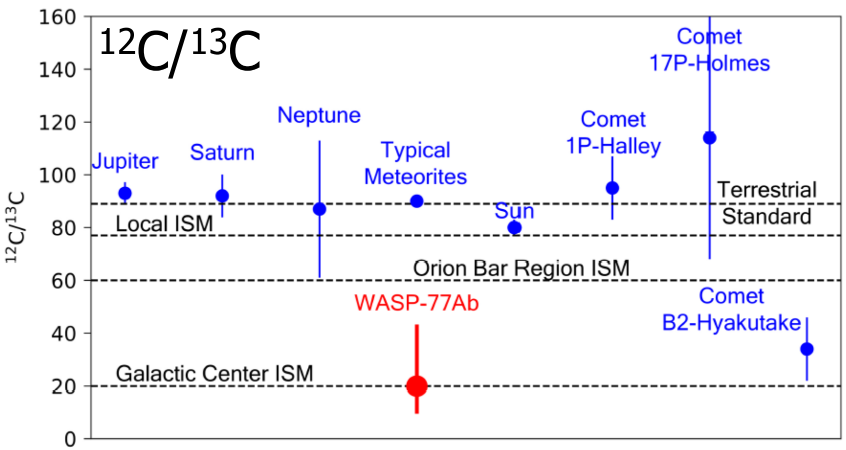
Characterize Exoplanetary Atmospheres

Gemini South/IGRINS, R~45,000

(Line+ 2021)







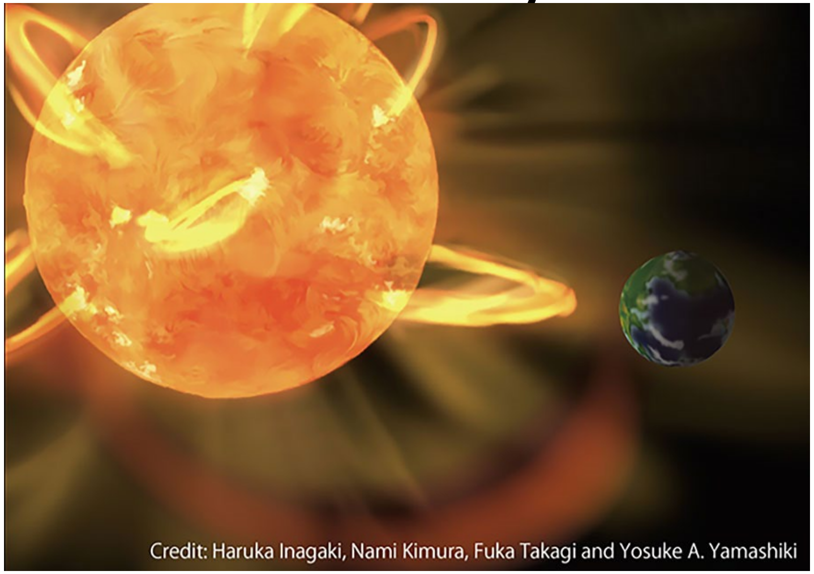
→ JWST, Ariel, GREX-PLUS, TMT/MODHIS, MICHI,...

Molecular composition, temperature profiles, etc..

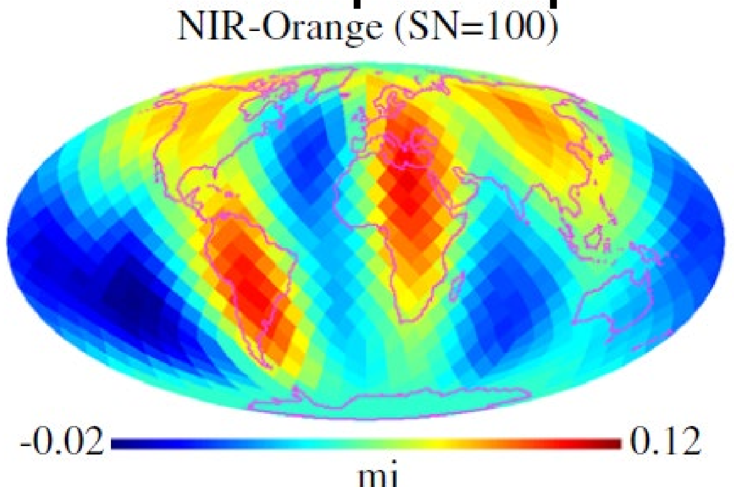
Habitable Worlds?

新学術 A paradigm shift by a new integrated theory of star formation

Effect of stellar flares on habitability?



Can we 'map' exoplanets?



(Fujii & Kawahara 2014)

→ TMT/PSI, ...

Ice chemistry
Isotope chemistry

Observations
Astronomy
exploration missions

Elemental abundances
Molecular snowlines
Nonthermal process

Microprocess
(Laboratory, Theory)
Physics, chemistry, spectroscopy

Models
Dynamical process
Chemical process

Summary

Origin of life? Possible diversity on exoplanets?

- Astronomical observations:
- broad band observations, high dispersion spectroscopy, collaboration with spectroscopists are important
- Collaborations with exploration mission are important
- Models: We need to think both global & local evolution of elemental abundances
- Ice chemistry model for COM formation should be improved, taking into account microprocesses
- Isotopes could be tracers of material evolution
- Evolution of snowlines is one of the keys for local evolution of elemental abundances
- Chemistry with nonthermal processes could be a key
- Molecular evolution model with dynamical process should be improved