



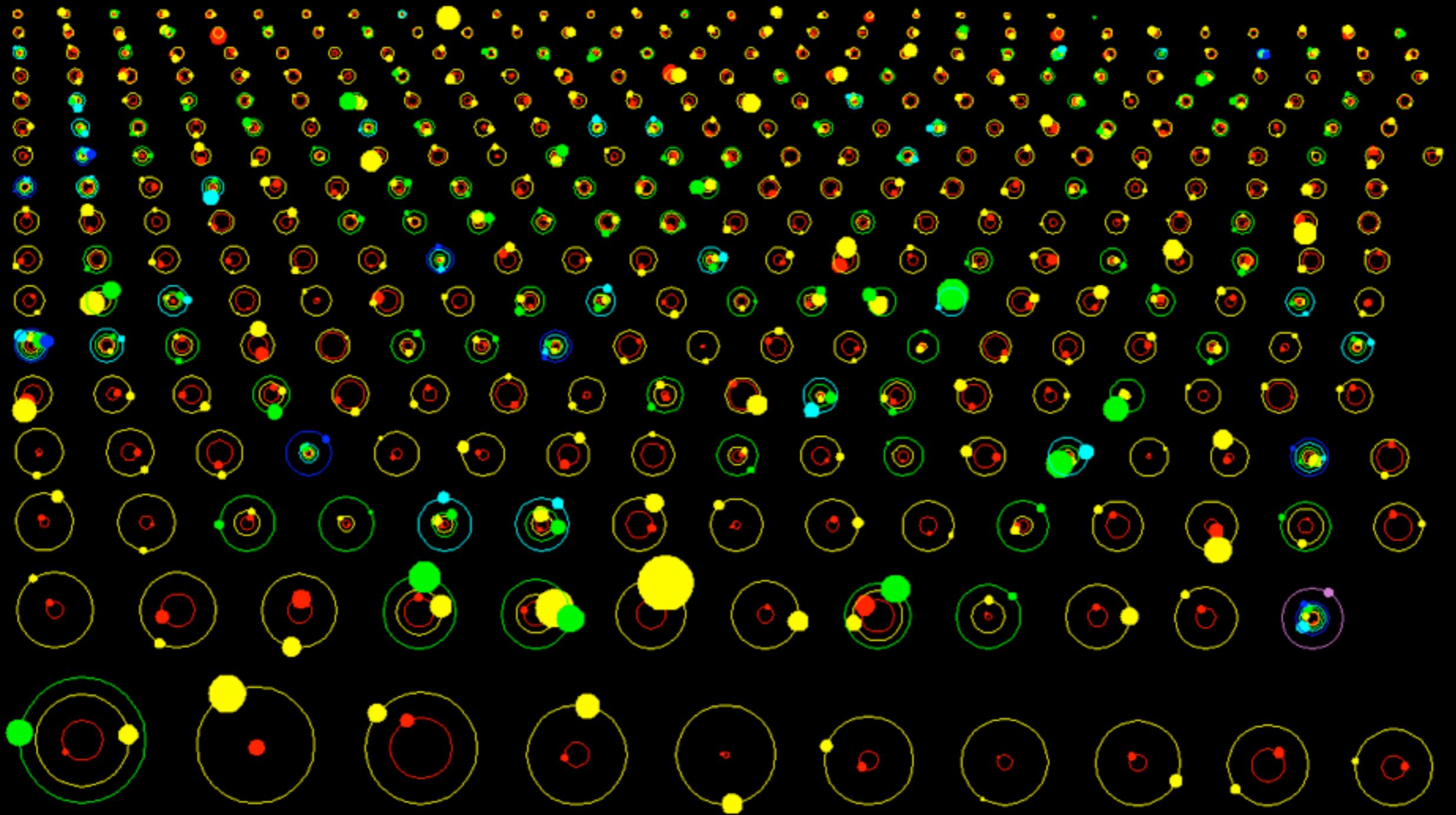
Explaining the  
Emergence of Life

Xander Tielens  
Sterrewacht Leiden

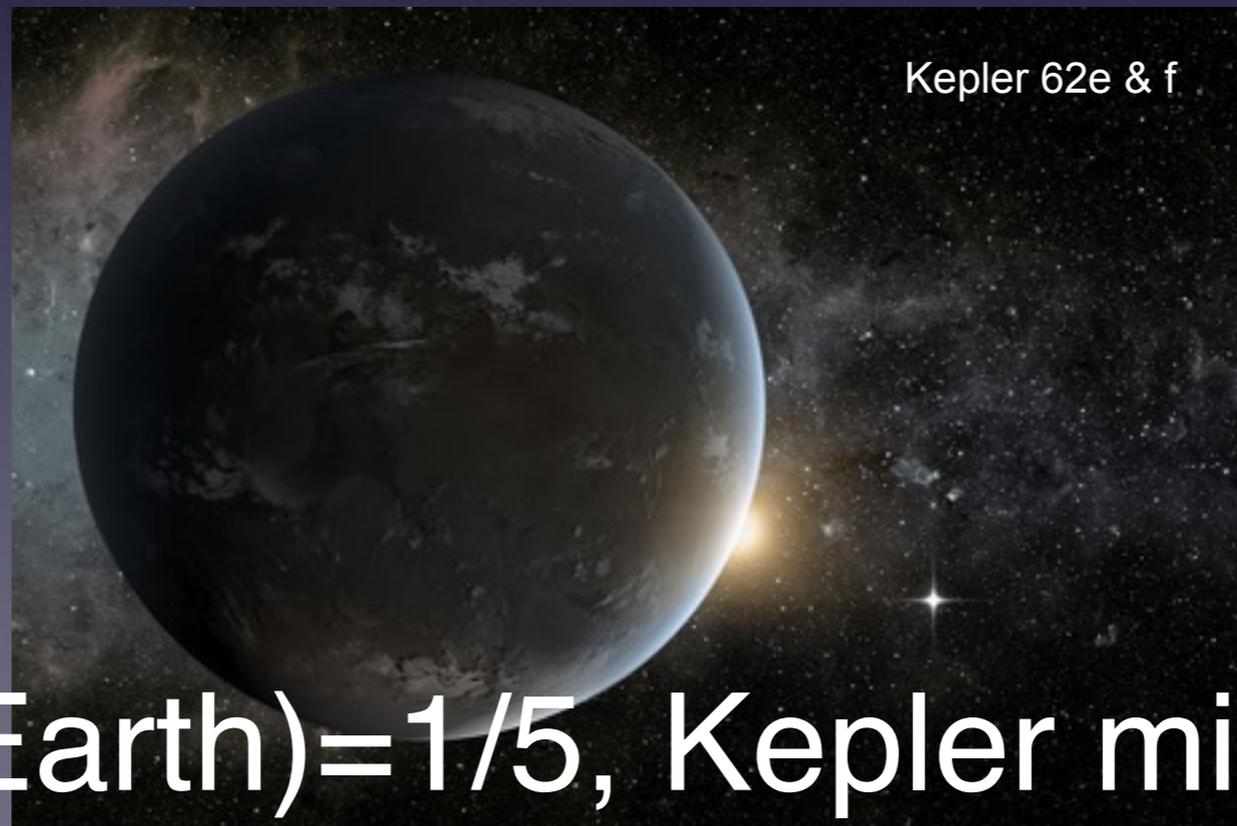
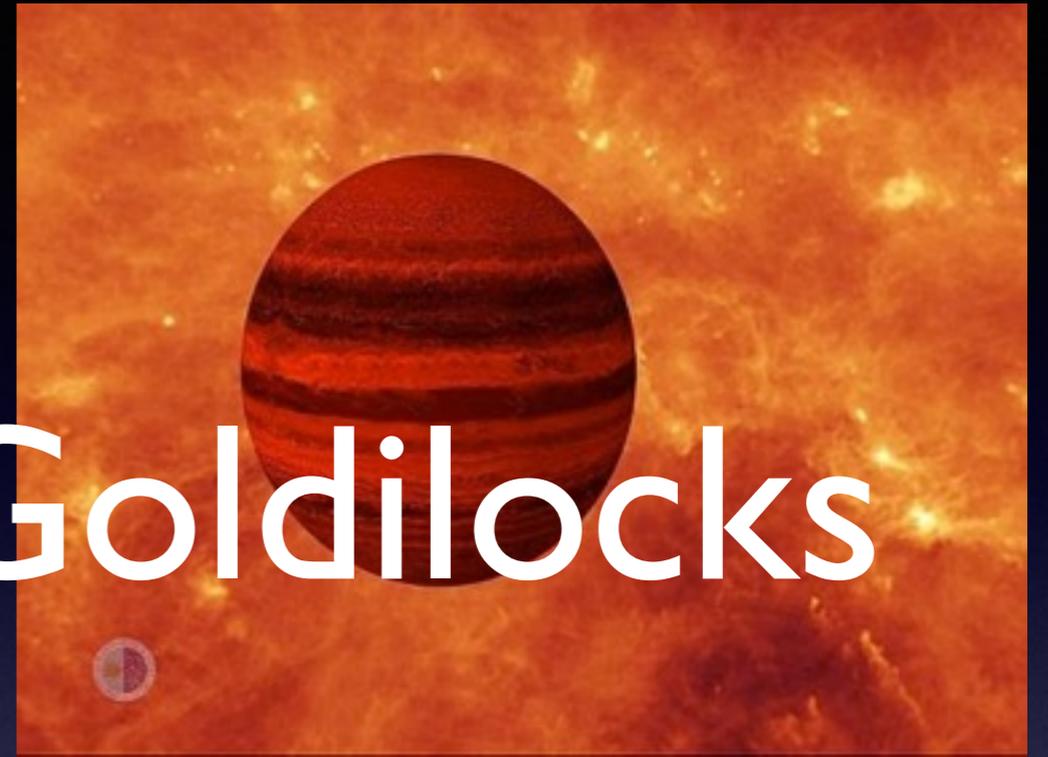
# The Kepler Orrery II

$t[\text{BJD}] = 2455879$

D. Fabrycky 2012

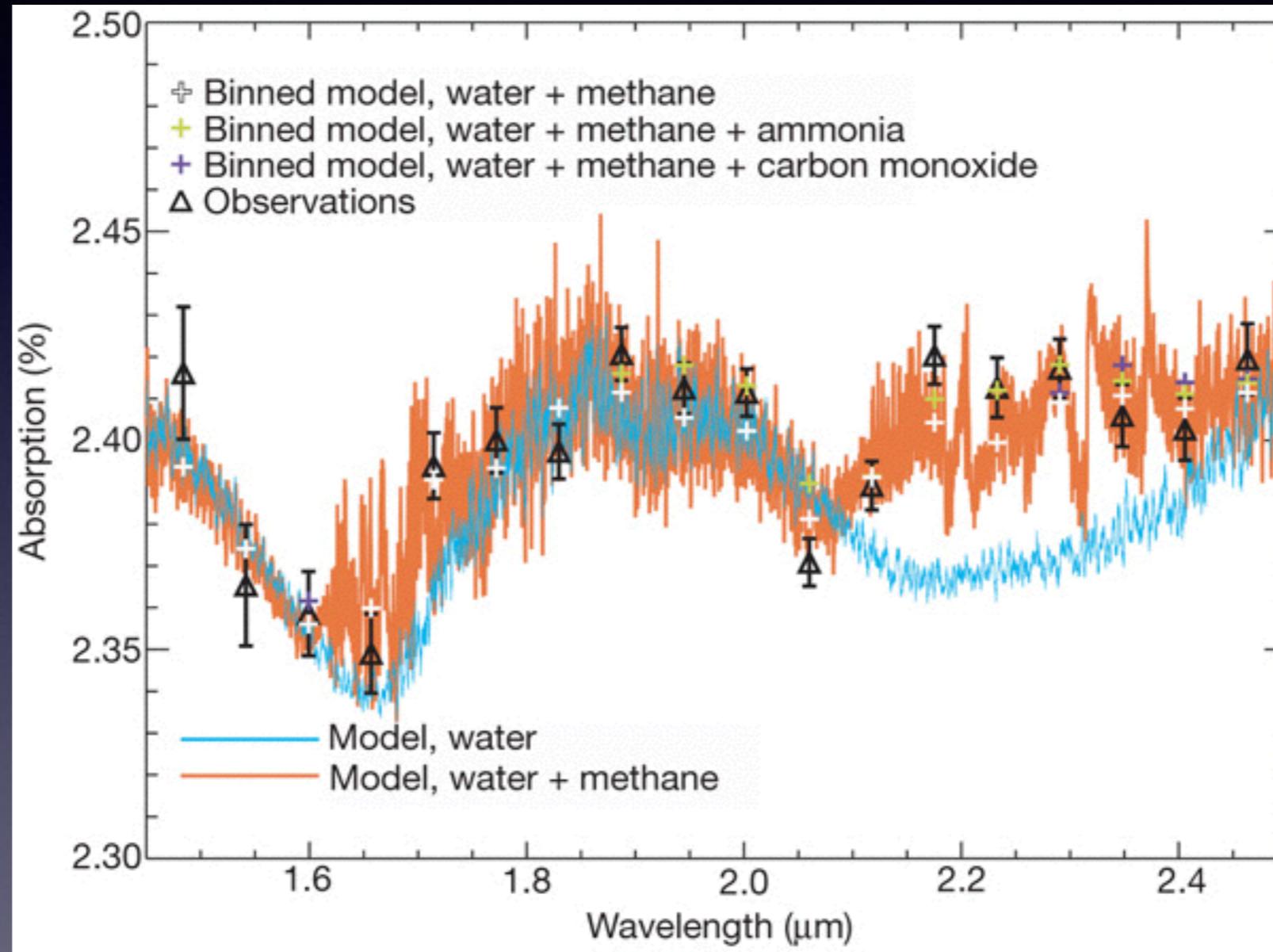


# Looking for Goldilocks



$\eta(\text{Earth})=1/5$ , Kepler mission

# Exoplanet atmosphere



# Hell on Earth



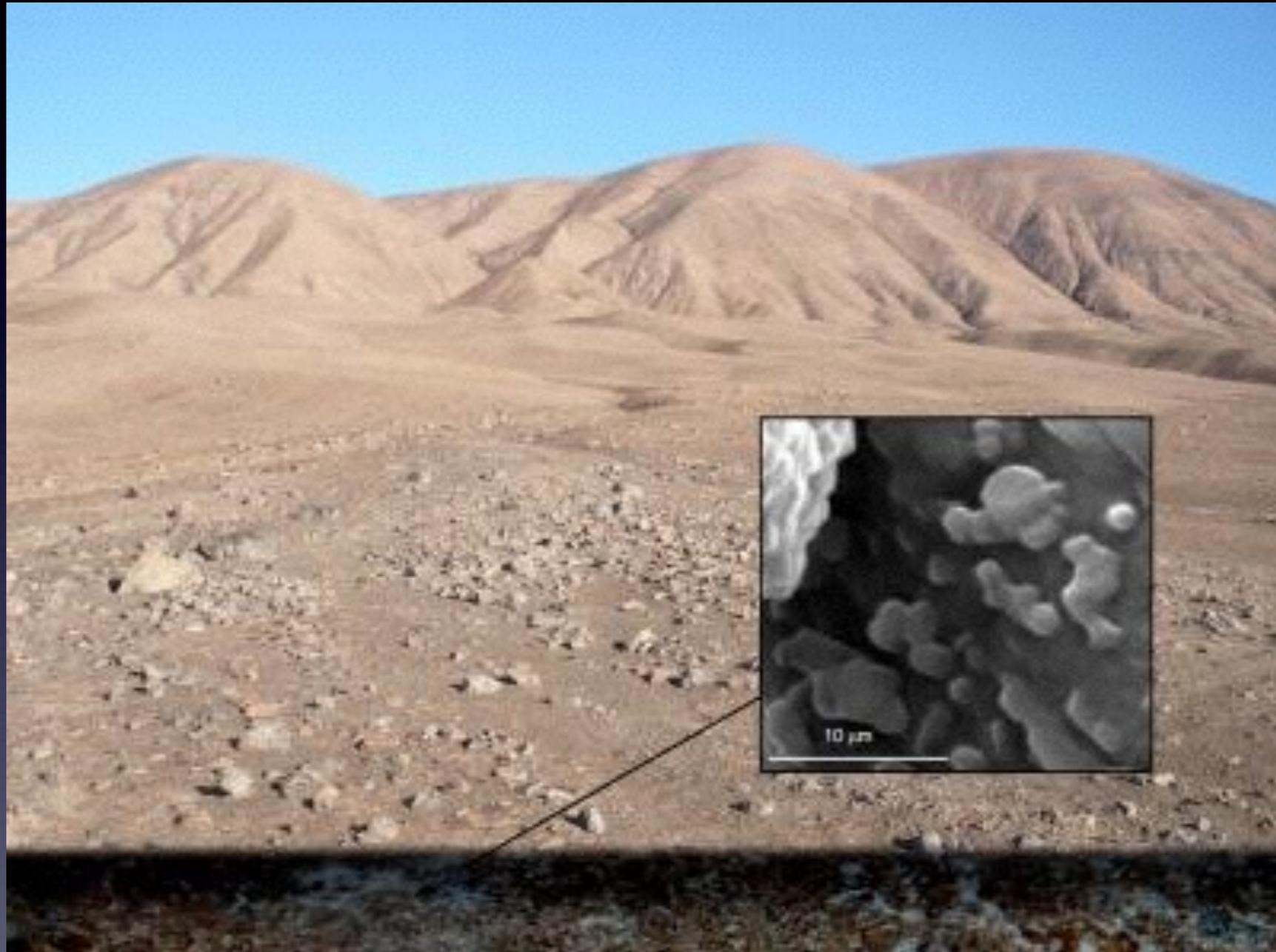
Cyano Bacteria in Grand Prismatic  
Spring Yellowstone

# Lakebed Fossils under the Ice

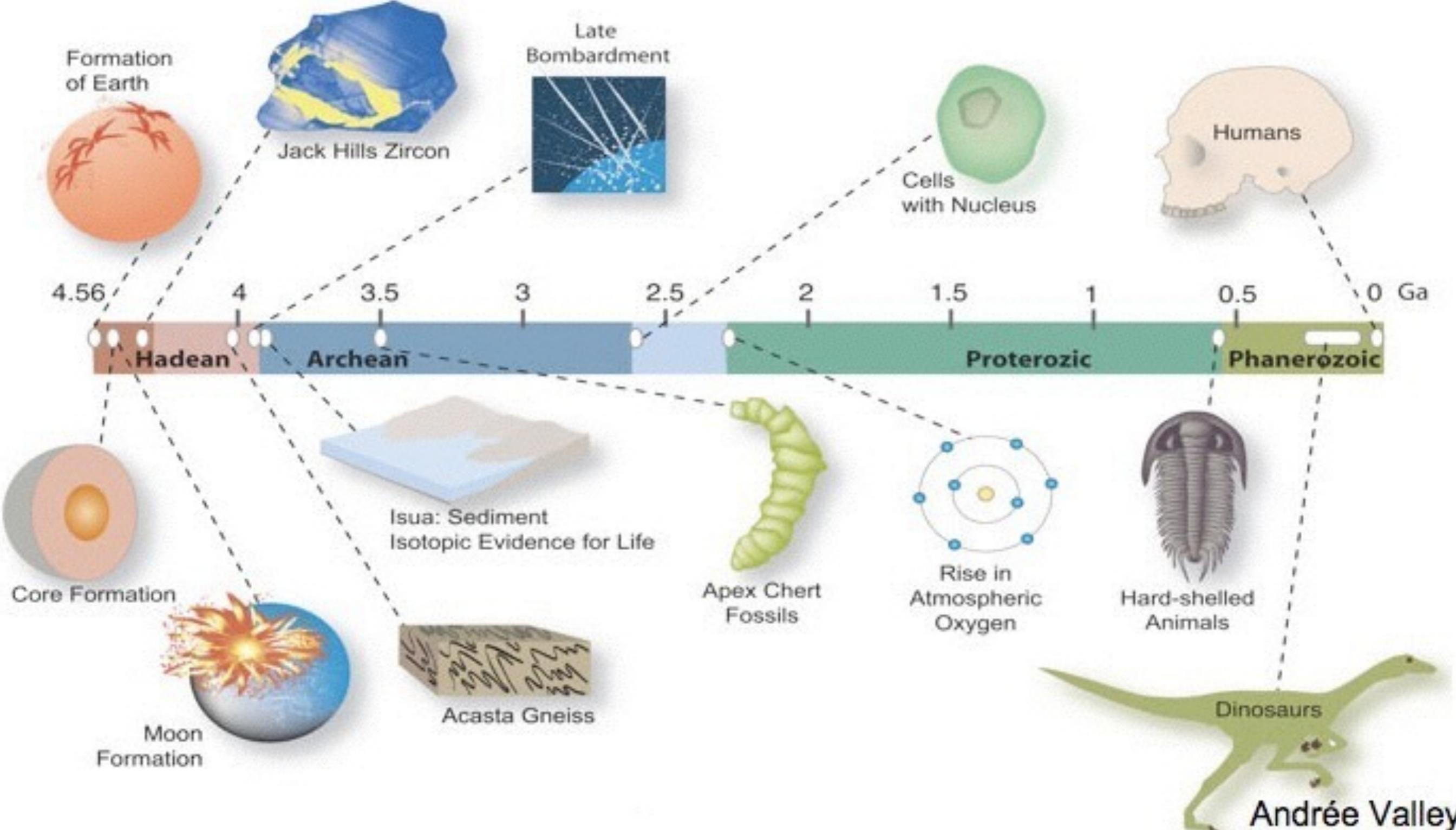


Bacterial colonies in Antarctica

# Life in the driest spot on Earth



Microbes grow on salt crystals in the Atacama desert

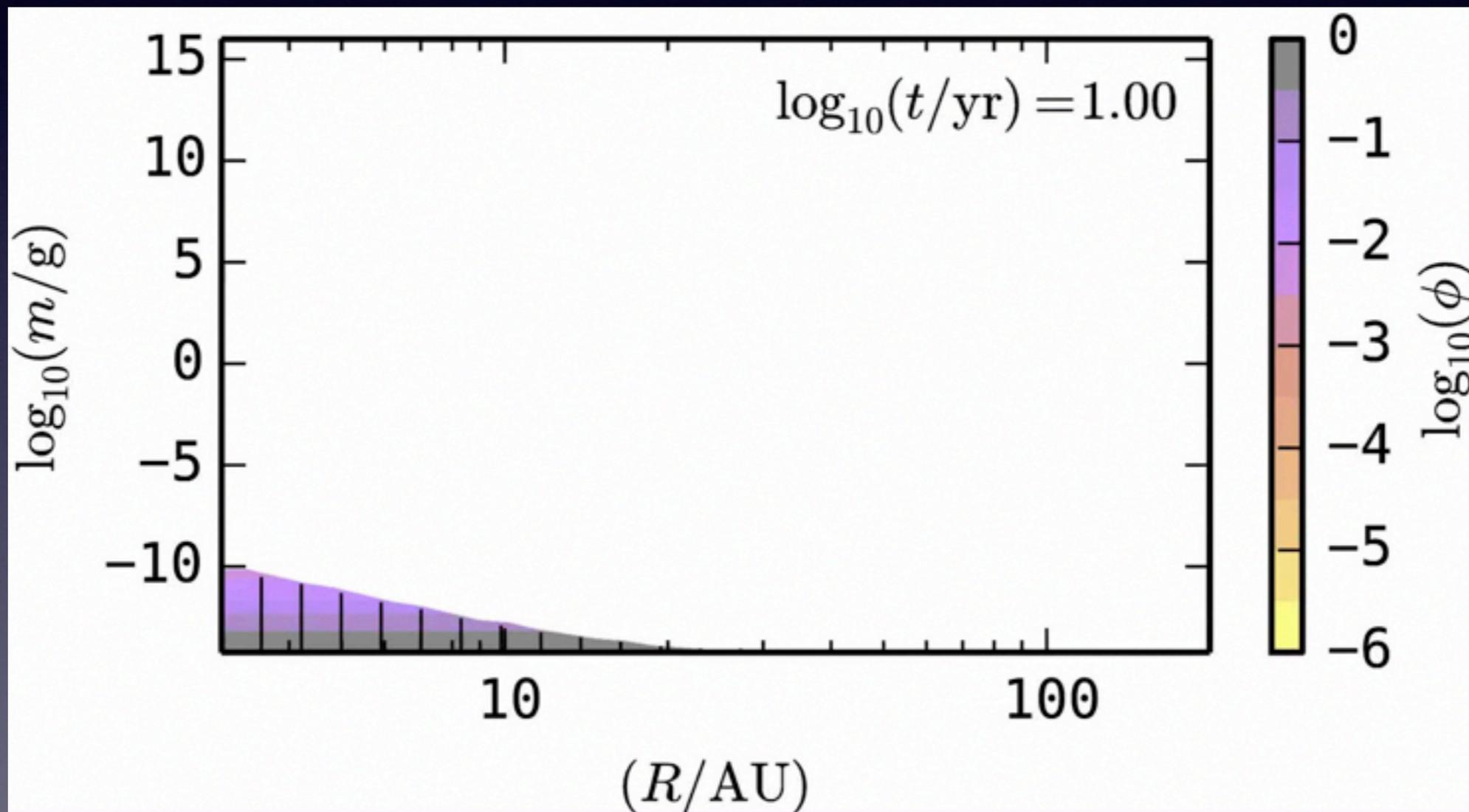


Life quickly evolved once the Solar System was formed

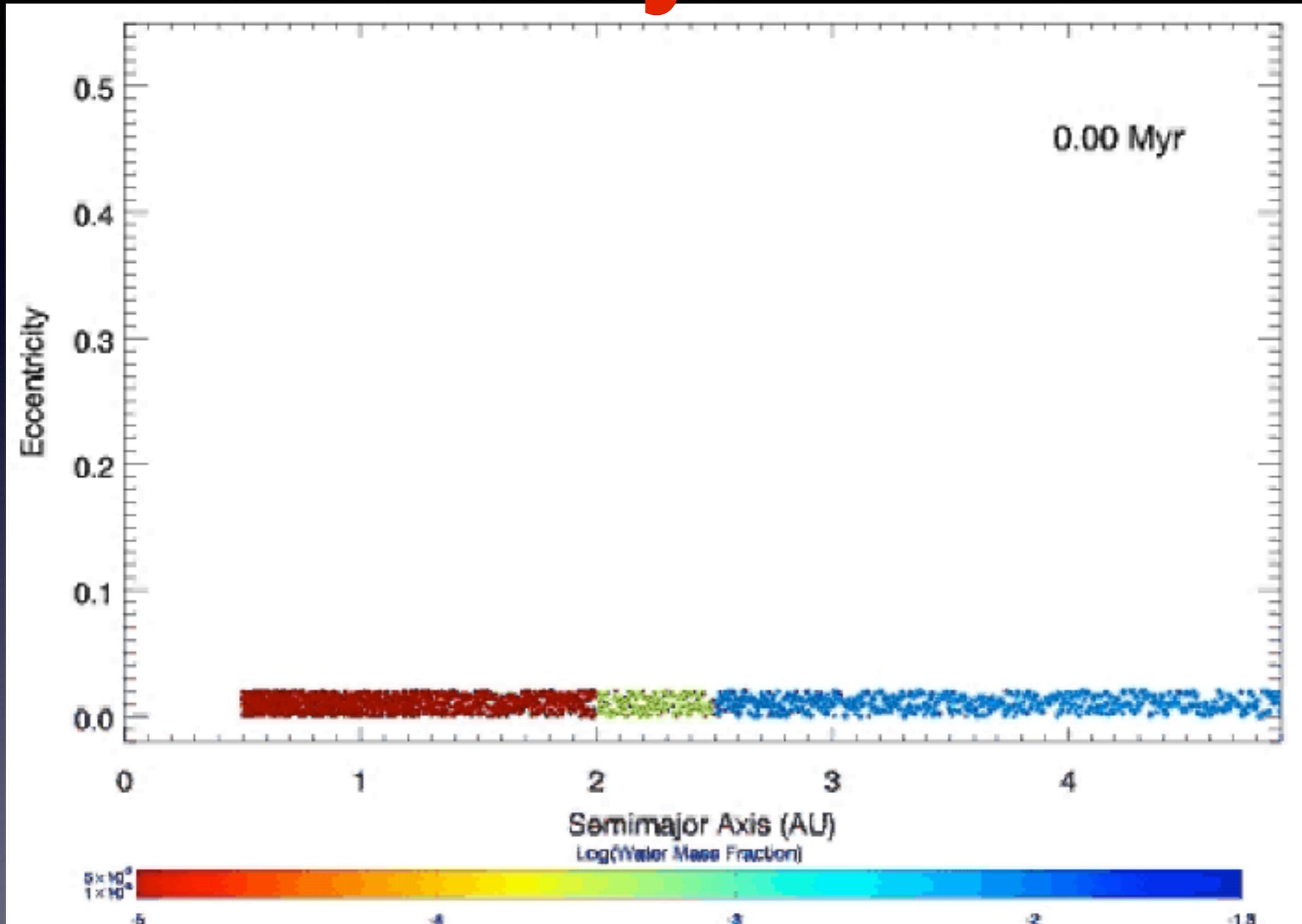
# Key Questions

- Building new worlds: What are the key processes in planet formation ? How do they depend on the environment ? What is the inventory of planets, particularly in the habitable zone ?
- Planetary habitats: What are the primordial sources of organics and volatiles and the processes that play a role in their formation and delivery ?
- Setting the stage for life: What are the conditions on the early Earth & newly formed planets and what are the key processes that set the stage for life ?

# Building Planetesimals One Grain at a Time



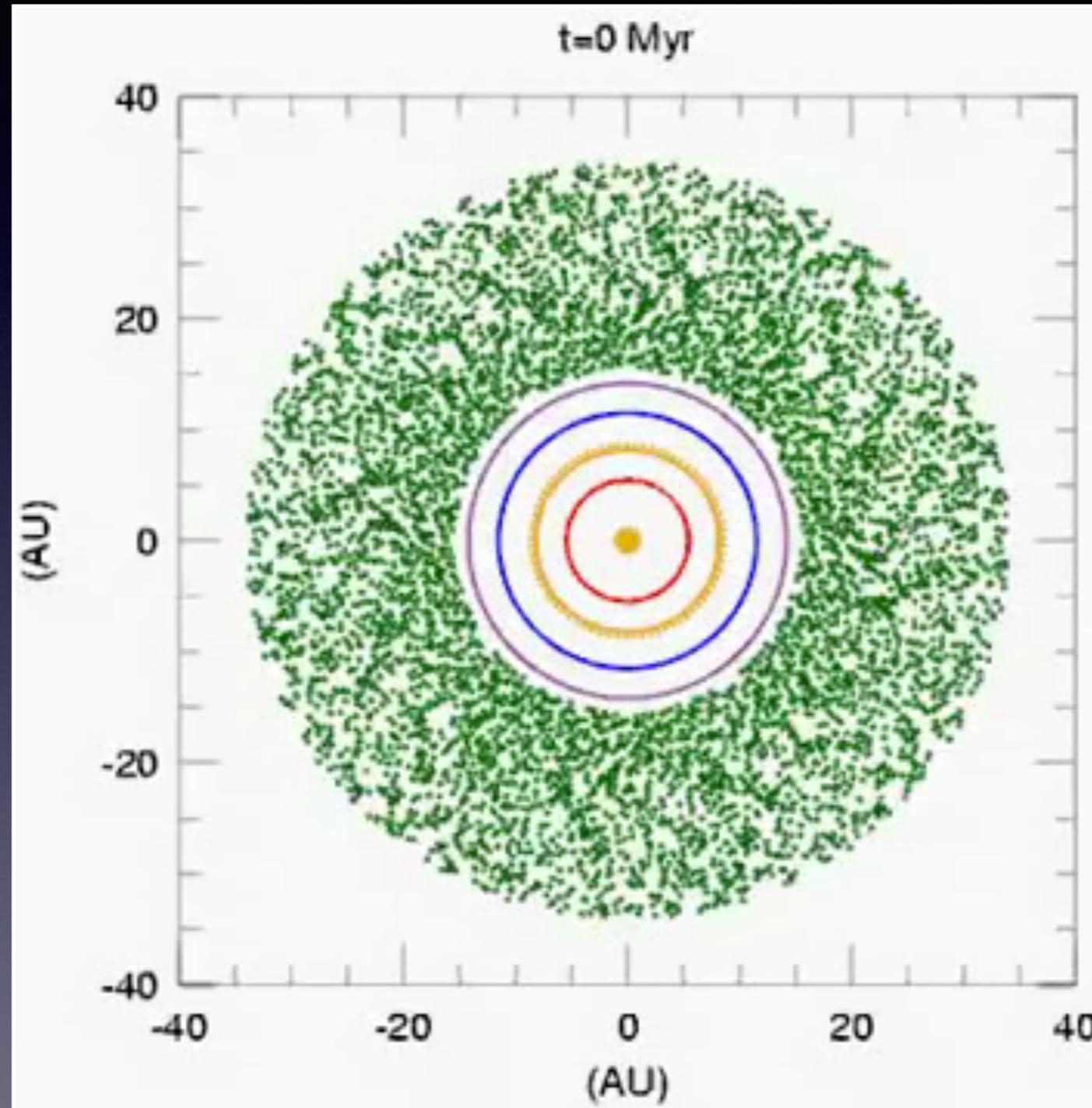
# From Embryo to Planet

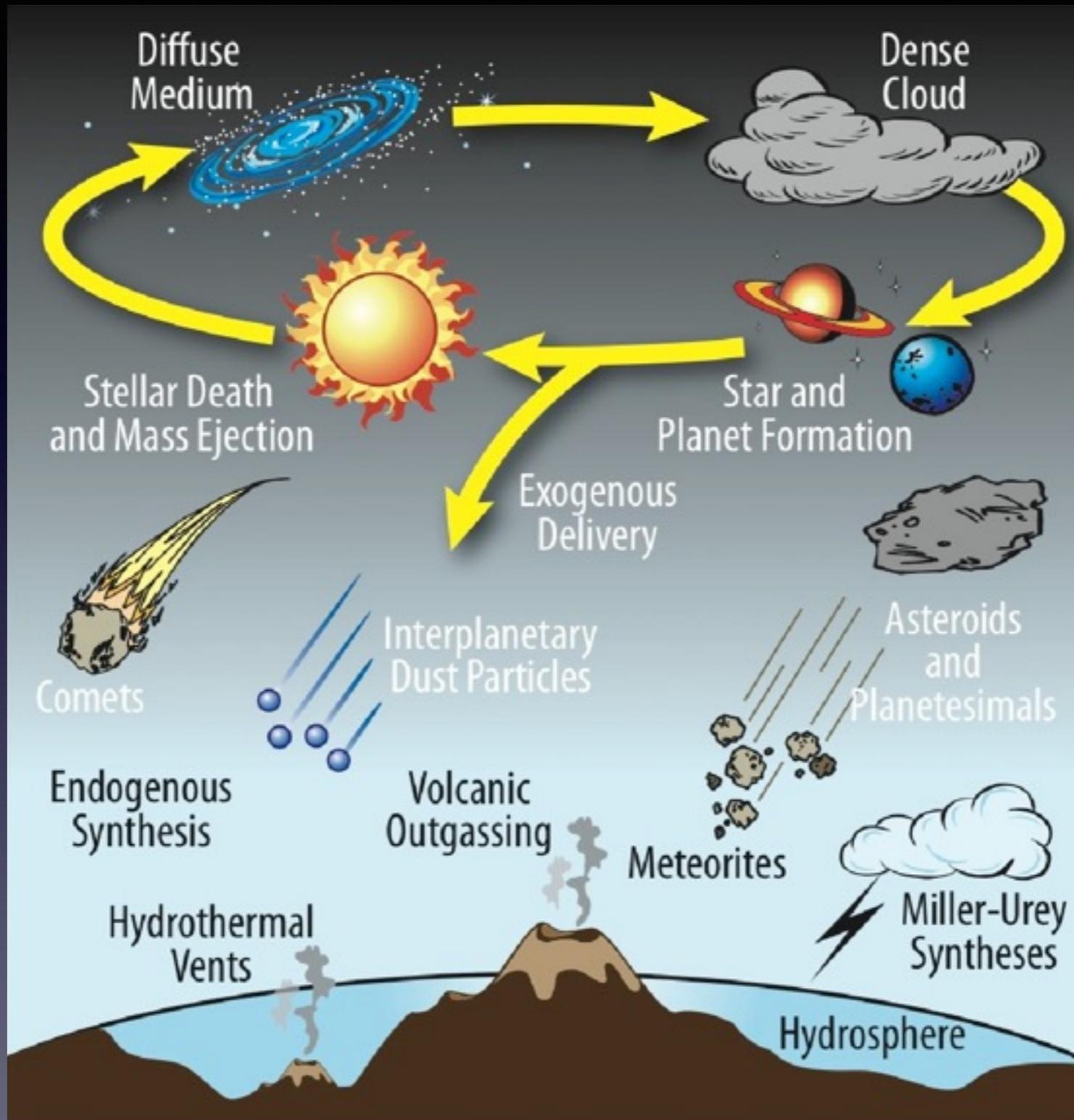


Petit et al, 2001, Icarus, 153, 338  
Raymond et al, 2004, Icarus, 168, 1

from embryo's to planets

# Late Heavy Bombardment

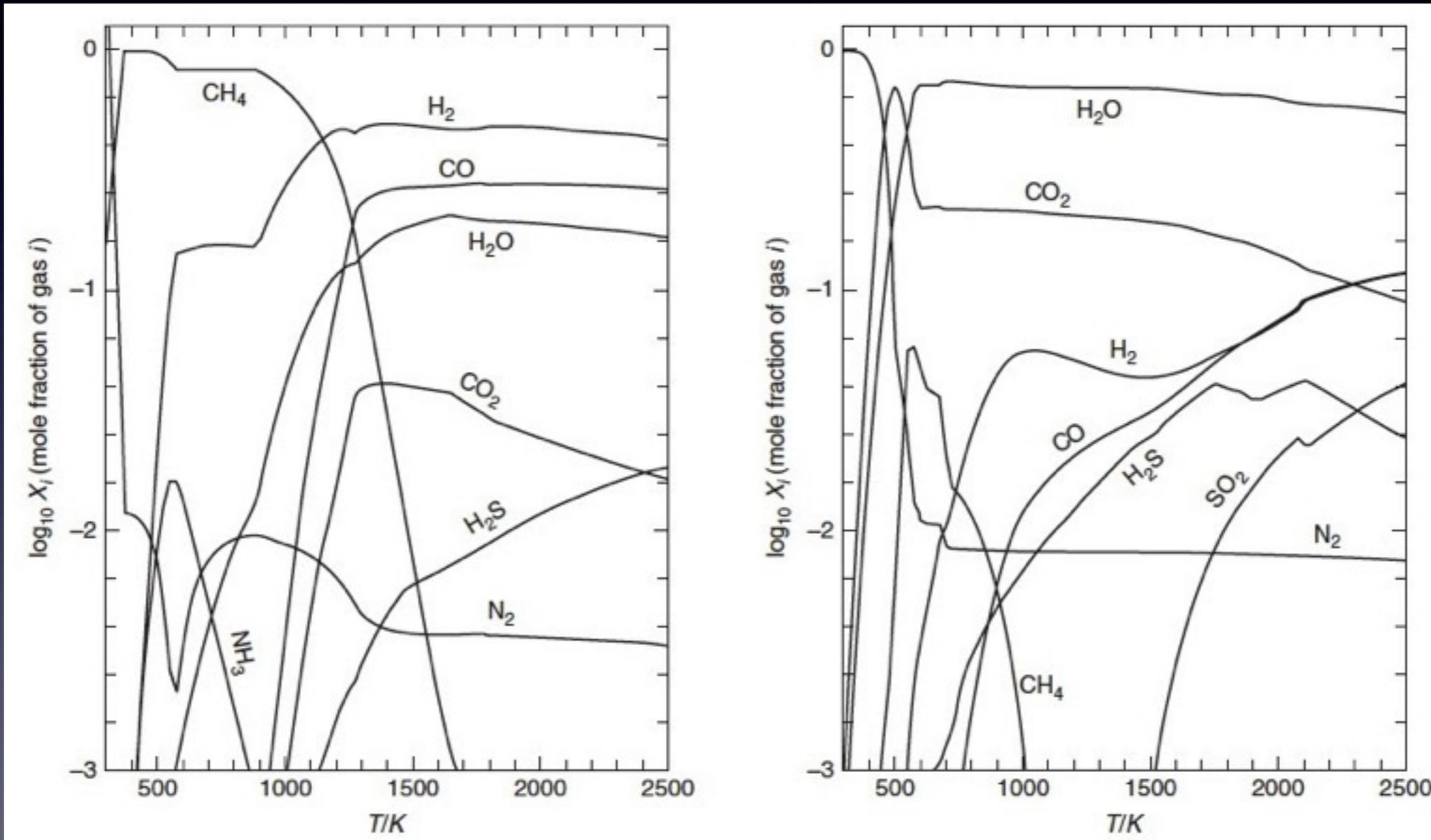




# Heritage Shows

“reduced” initial composition

“oxidized” initial composition

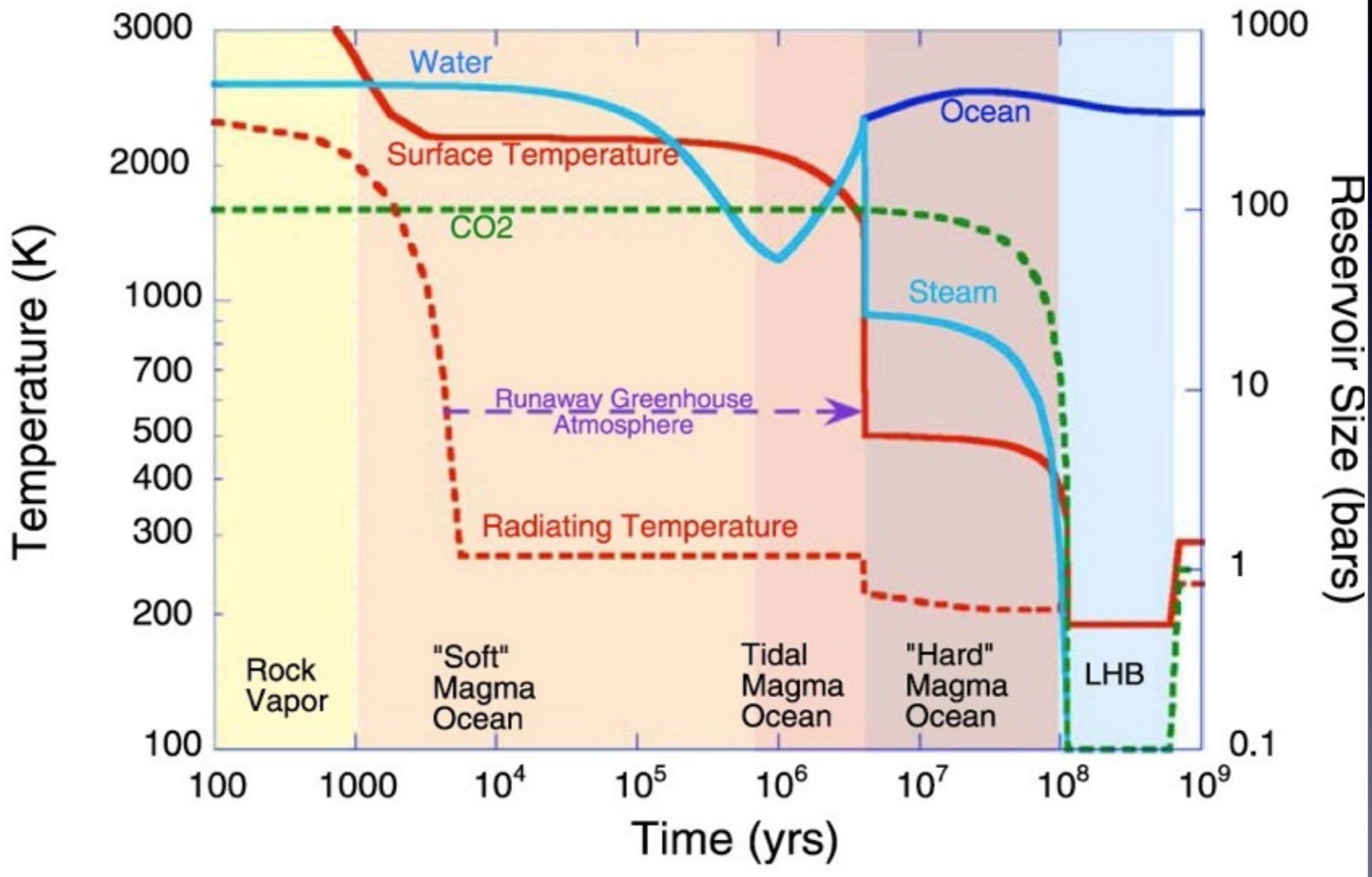


H chondrite

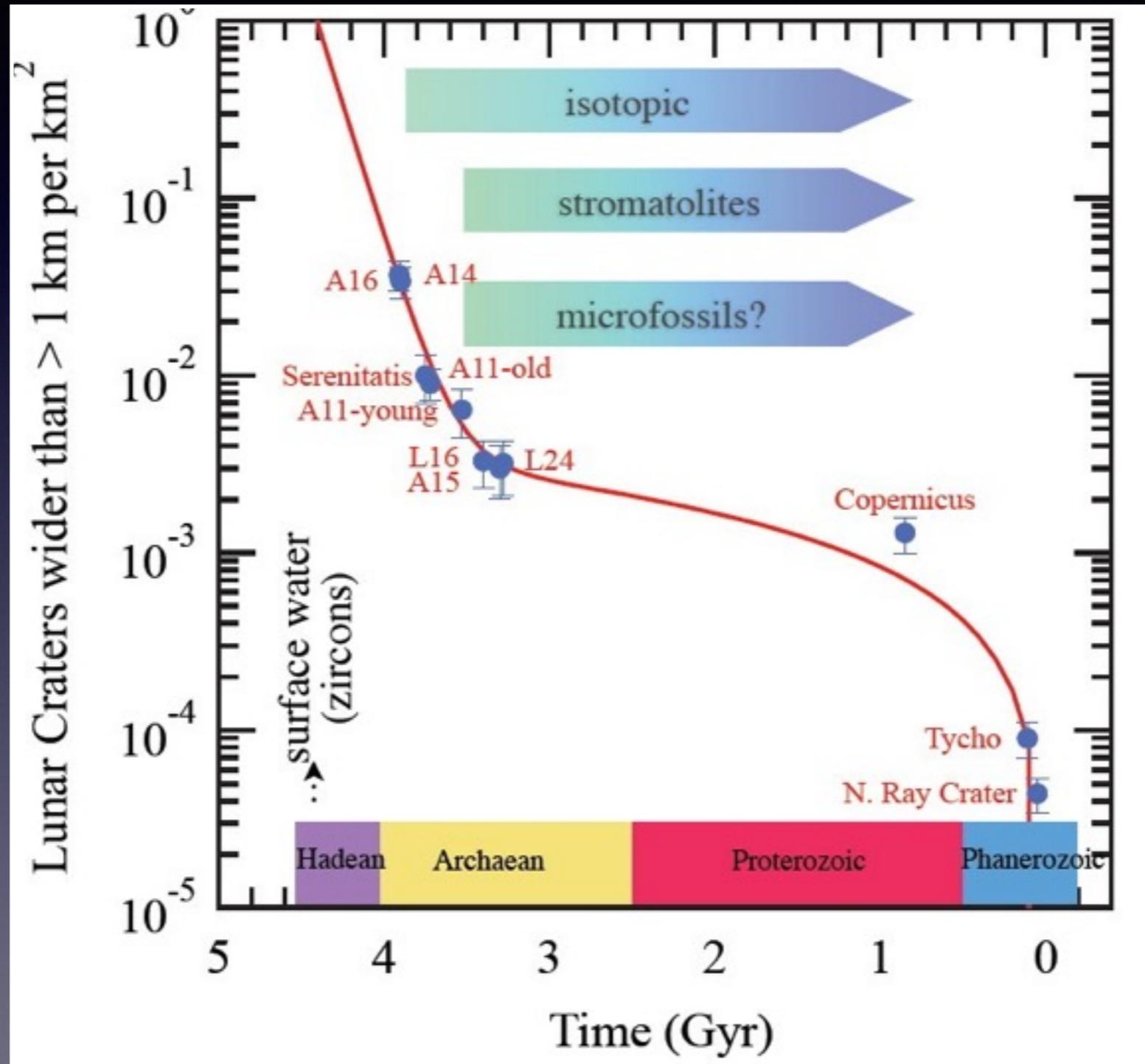
CI chondrite

# The Hadean Period

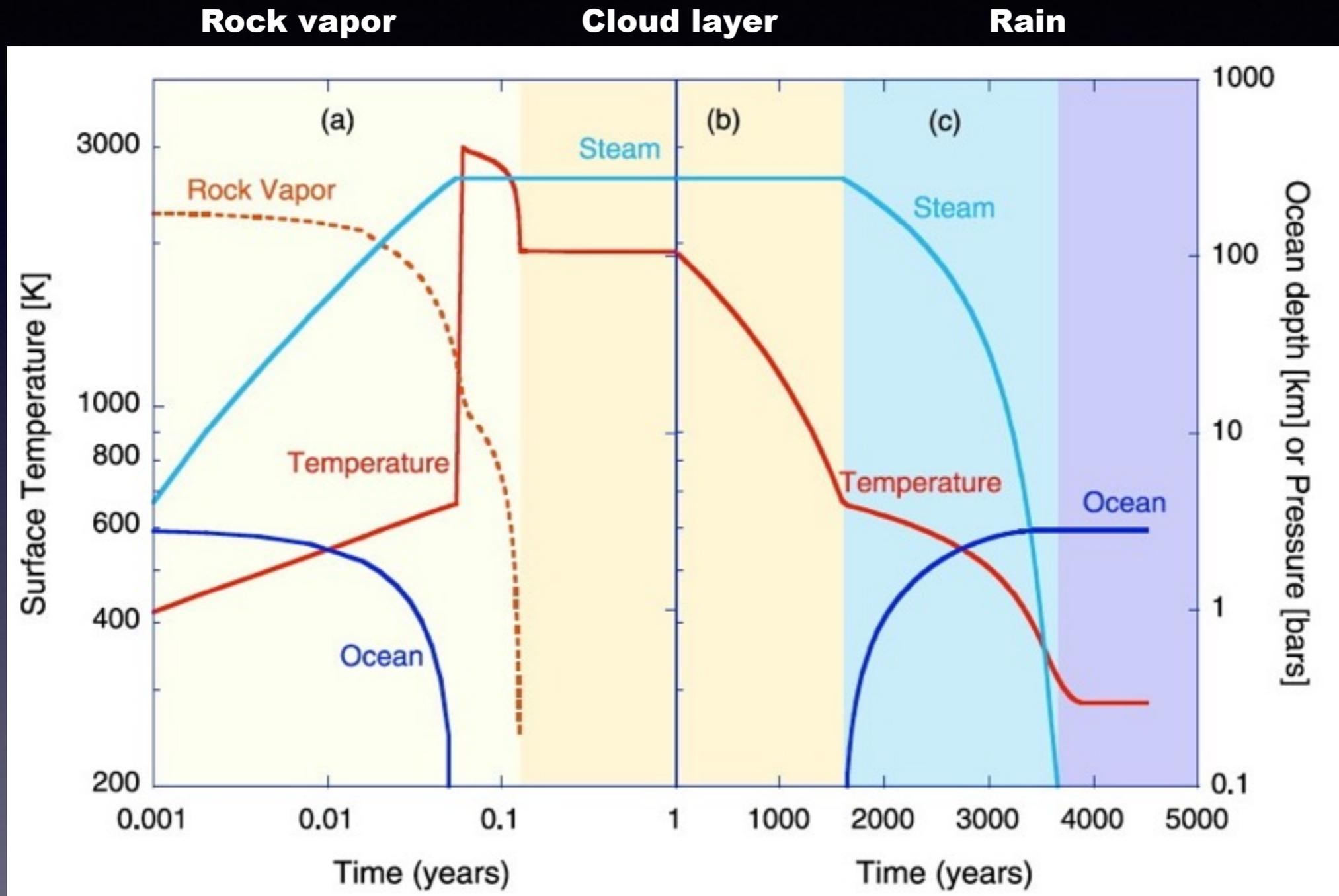
**Moon forming event**      **Magma ocean: H<sub>2</sub>O & CO<sub>2</sub> degassing**      **Warm, wet early Earth and subduction of CO<sub>2</sub>**



# Late Heavy Bombardment



# LHB: Ocean Vaporizing Impact



Zahnle et al, 2007, Spa Sci Rev, 129, 35



How did the Earth &  
Does life have an  
terrestrial planets get their  
interstellar heritage?  
volatile and organic inventory?

# Building the Solar System's Organic Inventory

From small  
to big



Protective  
environment of  
dense clouds

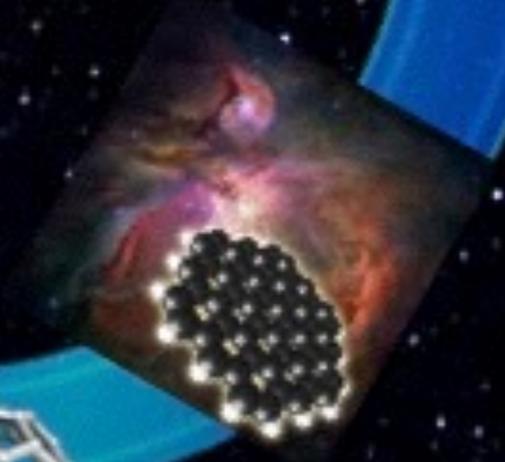
From big to  
small



Stars as sooting  
candles

Comets

Asteroids



Chemical growth: a  
few atoms at a time



UV and energetic  
particle processing

# Building the Solar System's Organic Inventory

## CO reservoir

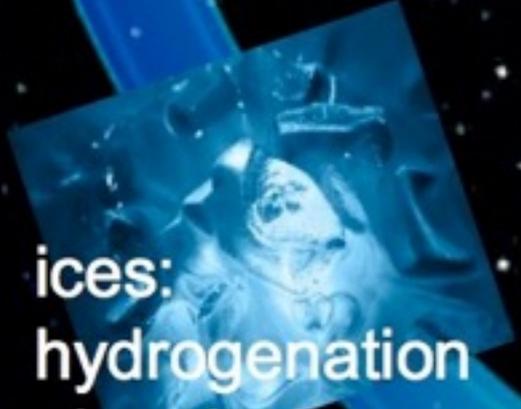


gas:  
ion-molecule reactions  
cosmic-ray photolysis

## PAH reservoir



stars:  
soot chemistry  
shock chemistry



ices:  
hydrogenation  
photolysis  
thermal polymerization  
ice-ion-molecule  
ice segregation

comets:  
energetic processing



asteroids:  
aqueous alteration

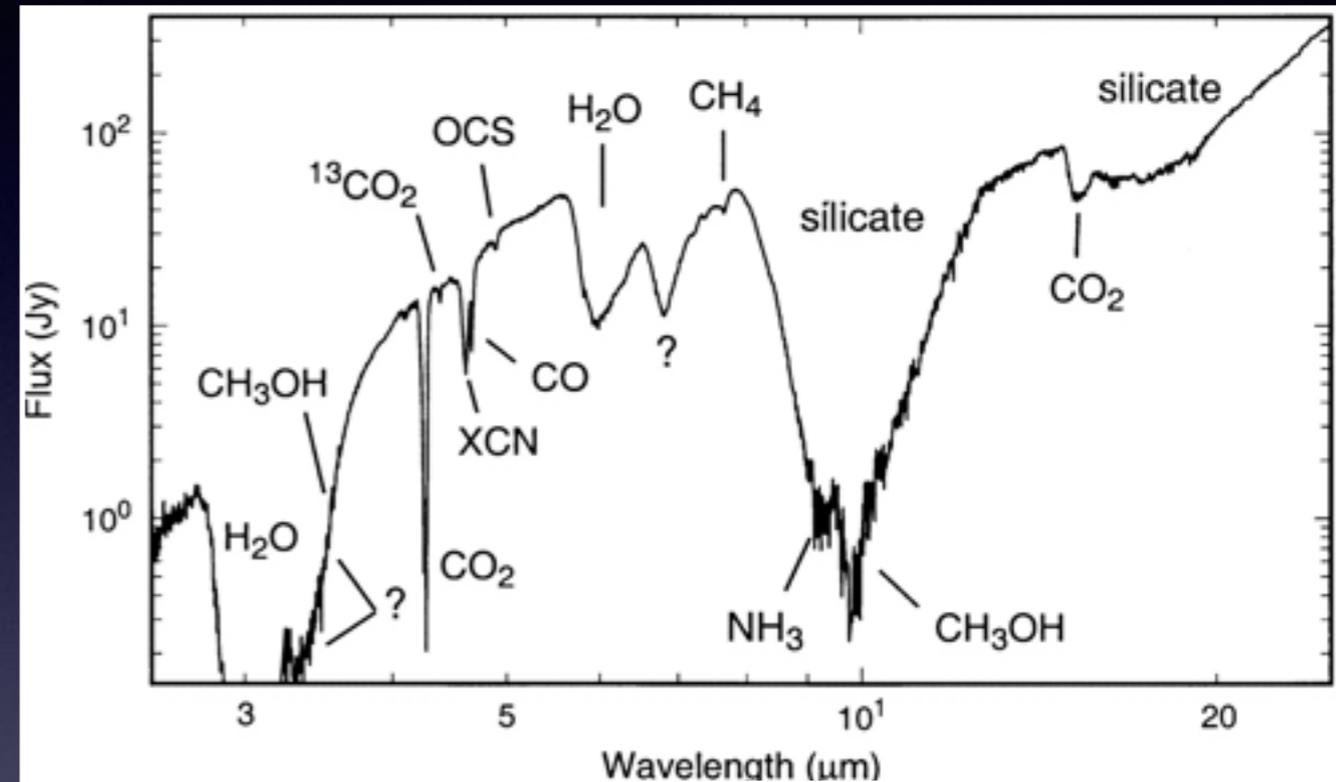
hot core:  
ice evaporation  
ion-molecule reactions

nebula :  
UV & X ray photolysis  
radical reactions  
hydrocarbon chemistry  
Fischer-Tropsch  
shocks, intermittent  
accretion, diffusion

Tielens 2011

# Gas-Grain Interaction

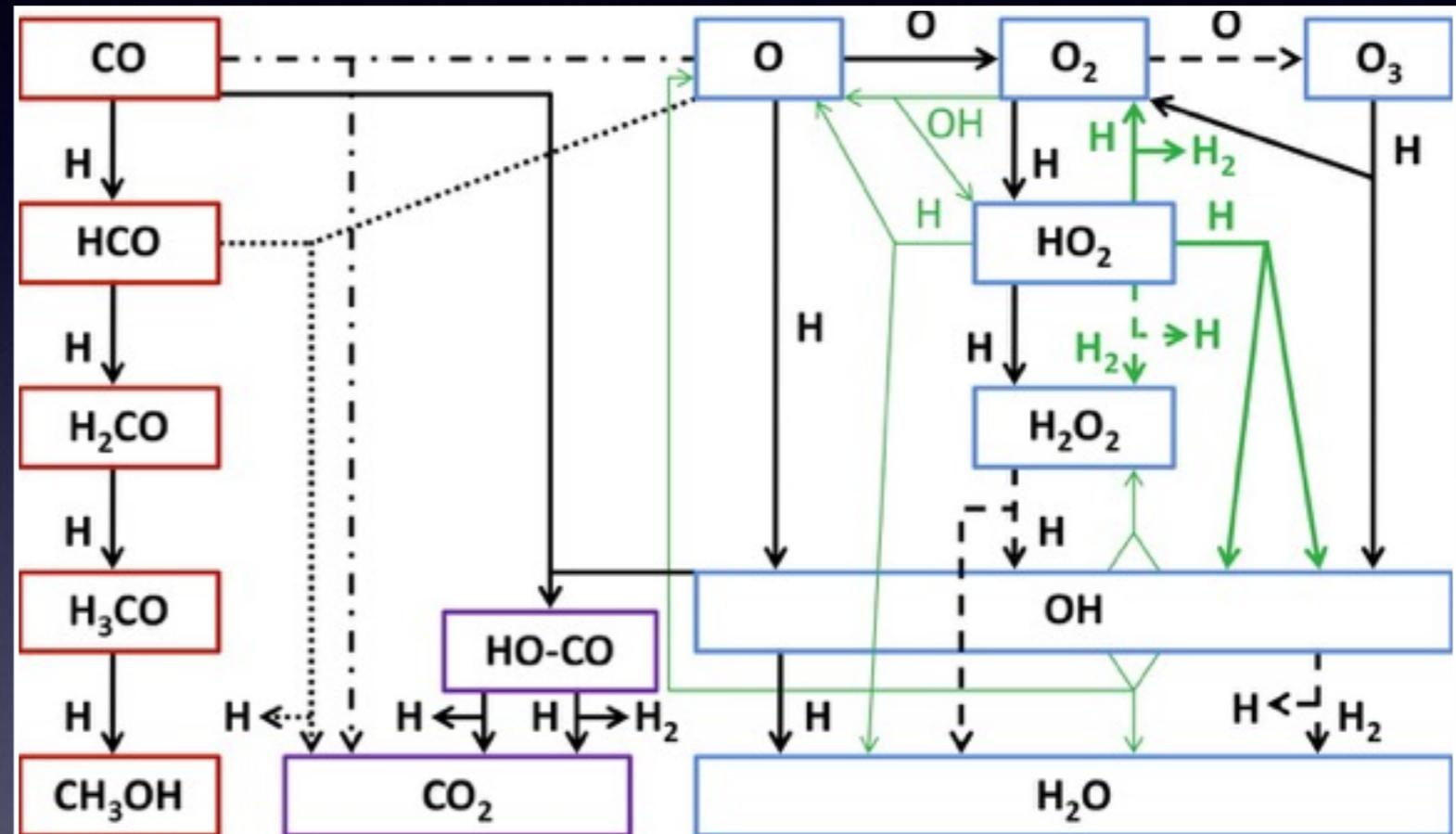
- Depletion in dense cores (i.e., B68)
- Interstellar ice
- Gas phase  $\text{HO}_2$  &  $\text{H}_2\text{O}_2$  (i.e., r Oph)
- High deuterium abundances of  $\text{CH}_3\text{OH}/\text{H}_2\text{CO}$  in protostellar envelopes
- Hot Core/Corino composition & deuterium fractionation



Caselli et al, 1999, ApJ, 523, L165 & Bergin et al, ApJ, 2001, 570, L101  
Gibb et al, 2004, ApJS, 151, 35; Boogert et al 2015, ARAA, 53, 541  
Parise et al 2012, A&A, 541, L11  
Praise et al, 2006, A&A, 453, 949  
Blake et al 1987, ApJ, 315, 621 & Ceccarelli et al, 2007, PPV, 47

# Grain Surface Reactions

- Hydrogenation & oxidation
- Tunneling
- Deuteration



H<sub>2</sub>CO/CH<sub>3</sub>OH

H<sub>2</sub>O

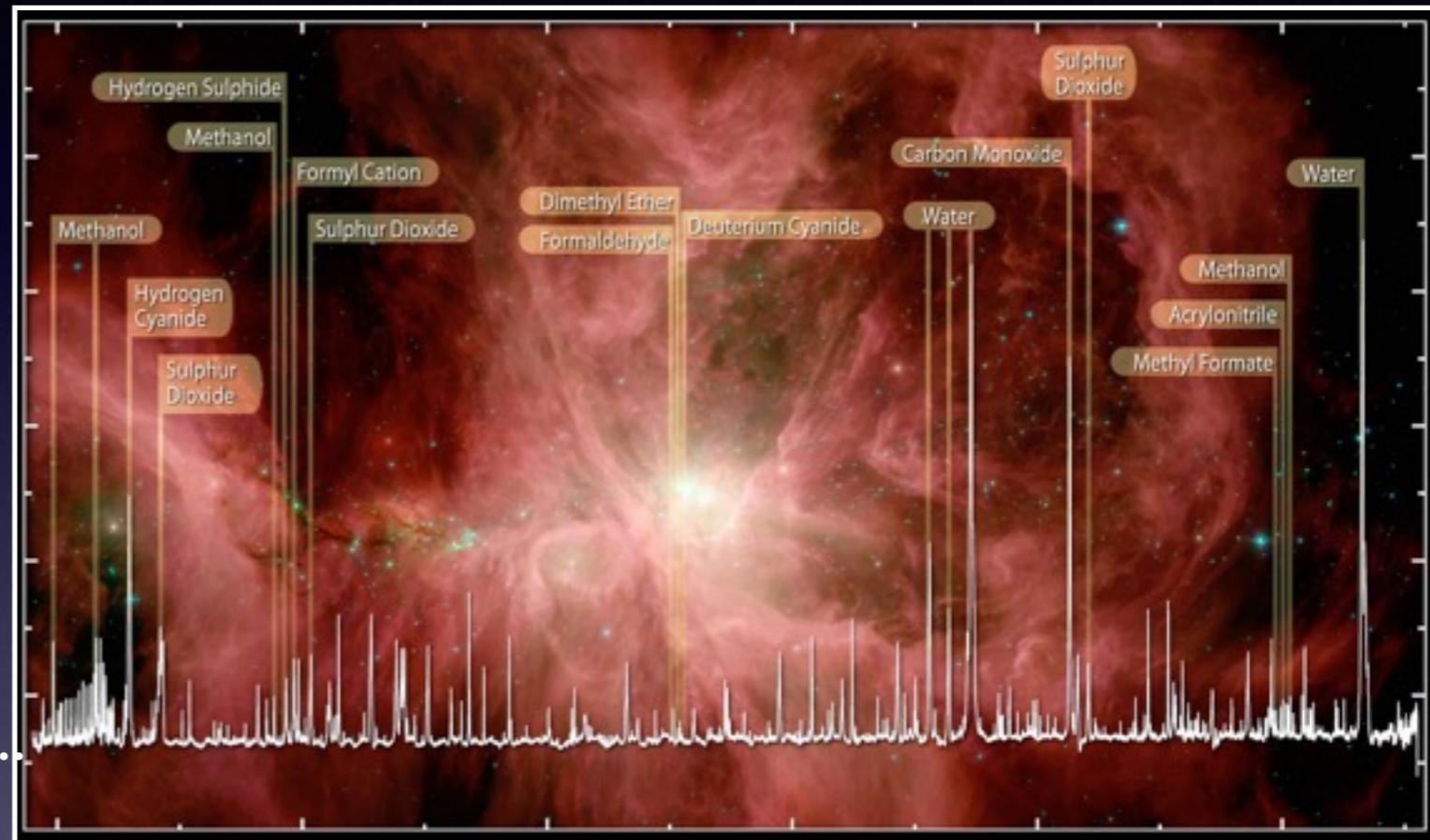
Tielens & Hagen, 1982, A&A, 114, 245

Fuchs et al 2009, A&A, 505, 629; Hidaka et al, 2004, ApJ, 614, 1124; 2009, ApJ, 702, 291; Hiraoka et al 1998, ApJ, 498, 710; Ioppolo et al., 2008, ApJ, 686, 1474

Ioppolo et al., 2008, ApJ, 686, 1474; Dulieu et al 2010, A&A, 512, A30; Hiraoka et al 1998, ApJ, 498, 710; Miyauchi et al 2008, Chem Phys Lett, 456, 27; Mokrane et al, 2009, ApJ, 705, L195

# Simple Organic Molecules (“SOM”)

- Warm dense gas with rich organic inventory: of relatively simple organic molecules
  - $\text{CH}_3\text{OH}$ ,  $\text{CH}_3\text{CH}_2\text{OH}$ ,  $\text{CH}_3\text{OCH}_3$ ,  $\text{H}_2\text{CO}$ ,  $\text{CH}_3\text{CHO}$ ,  $\text{HCOOH}$ ,  $\text{NH}_2\text{CHO}$ , ...
  - $\text{HCN}$ ,  $\text{CH}_3\text{CN}$ ,  $\text{CH}_3\text{CH}_2\text{CN}$ , ...
- Large deuterium fractionations
- Driven by evaporation of ice mantles formed in cold phase



# Origin of “SOM”

Deuterium fractionation implies formed from cold-reservoir-progenitors

- Surface chemistry in cold regions
- Photolysis of ices
- Evaporation followed by gas phase reactions
- Ion molecule chemistry in ices

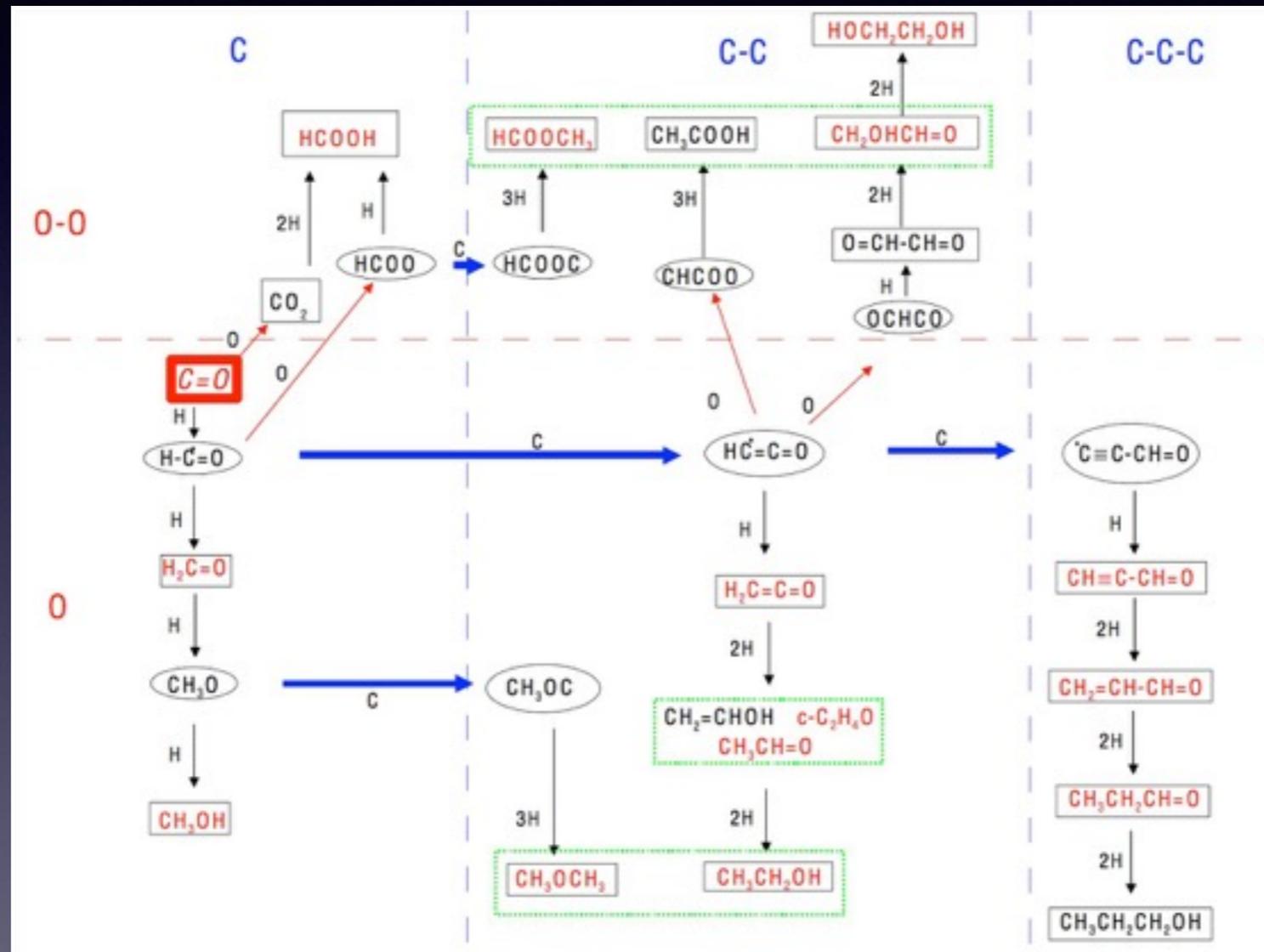
Gas phase chemistry: Charnley et al 1992,ApJ, 399, L71, Caselli et al, 1993,ApJ, 408, 538; Geppert et al, Faraday discussions, 133, 177, Horn et al, 2004,ApJ, 611, 605

Grain surface chemistry: Charnley & Rodgers 2007 Bioastronomy

Charged ices: Bouwman et al, 2011, A&A, 529, 46; Schutte et al, 2003, 398, 1049; Demyk et al, 1998, A&A, 339, 553, Balog et al 2009, Phys Rev Lett, 201, 73003

Photolyzed ices: Garrod et al, 2008, ApJ, 682, 283; Oberg et al, 2010, ApJ, 718, 832

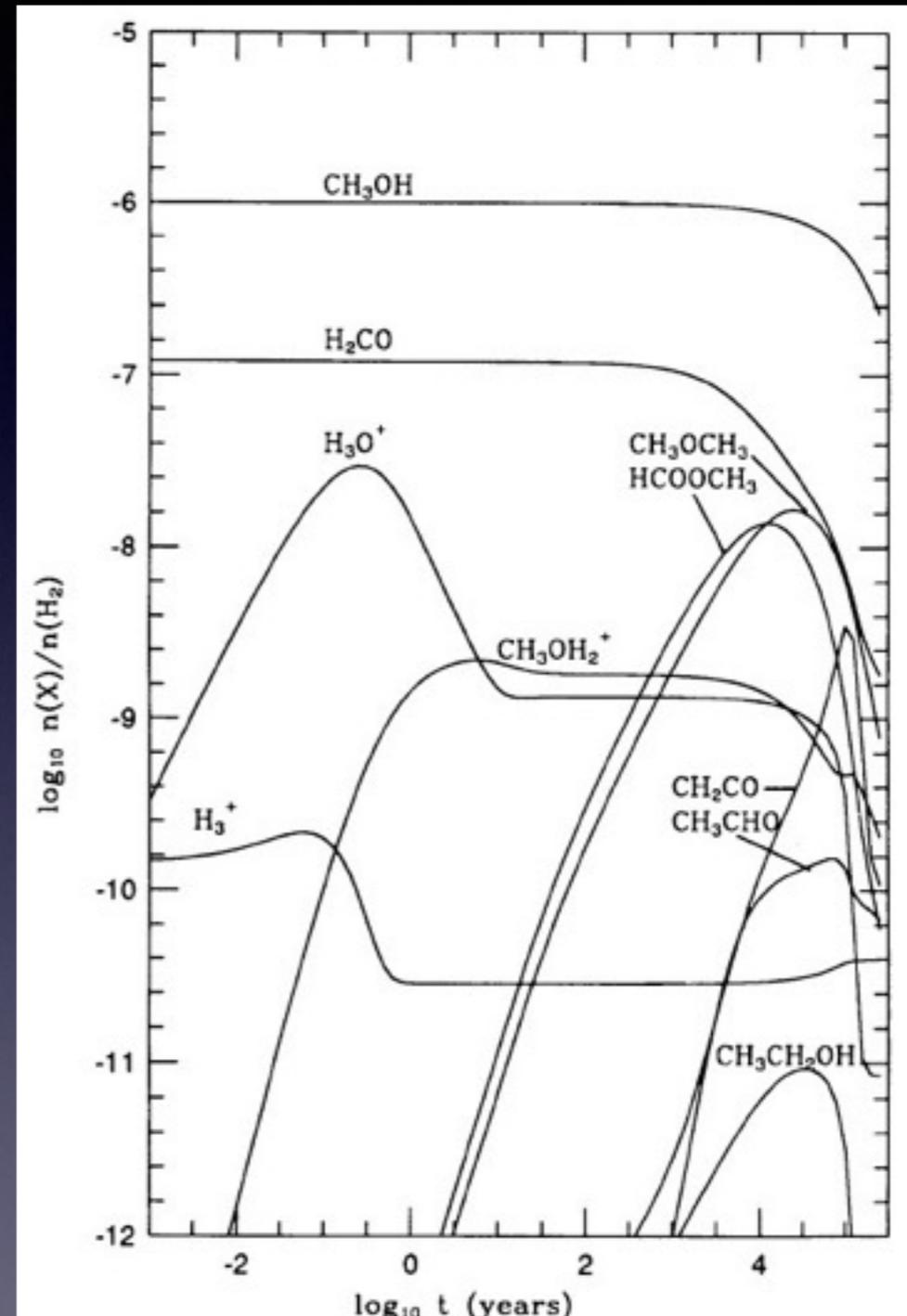
# Grain Surface Chemistry



“SOM” molecules require ‘free’ carbon

# Evaporating Ices

- Evaporating ice molecules drive rich chemistry
- Protonated methanol & methyl transfer
- Issues:
  - Experimental studies disagree
    - formation of intermediaries inhibited
    - Recombination leads to fragmentation
    - Role of ammonia as proton scavenger
  - Chemical clock  $\sim 3 \times 10^4$  yr incompatible with hot corinos



Charnley et al 1992, ApJ, 399, L71

Caselli et al, 1993, ApJ, 408, 538

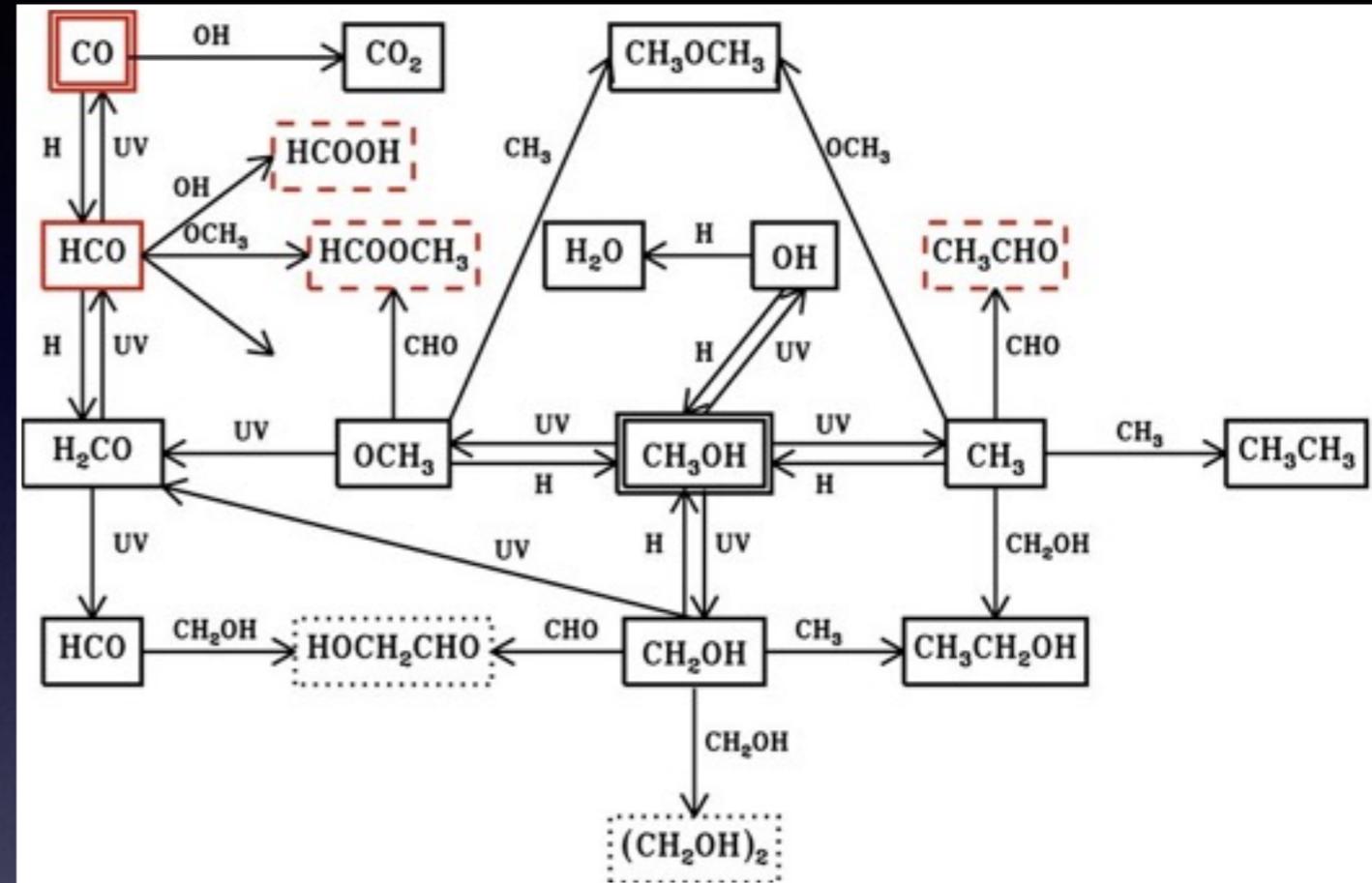
Geppert et al, Faraday discussions, 133, 177

Horn et al, 2004, ApJ, 611, 605

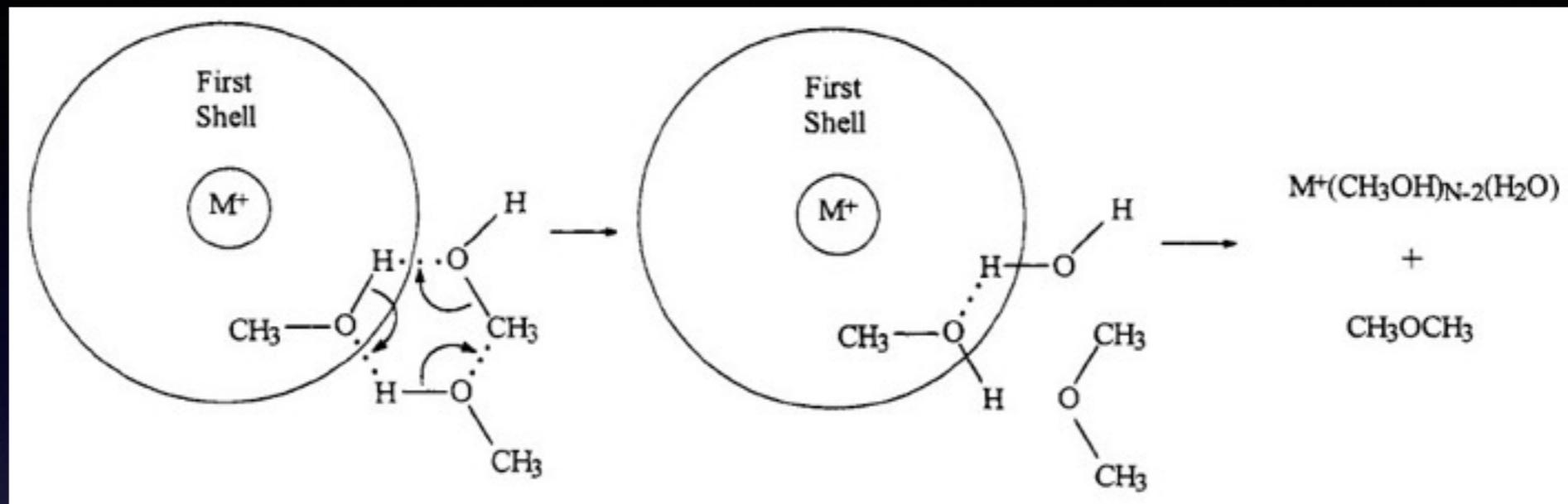
# Photolyzed Ices

UV photolysis/ion bombardment & warm up

- Radical production ( $\text{CH}_3$  & others)
- Recombination
- Issues:
  - Chemical specificity
  - Polymerization



# Charged Ices

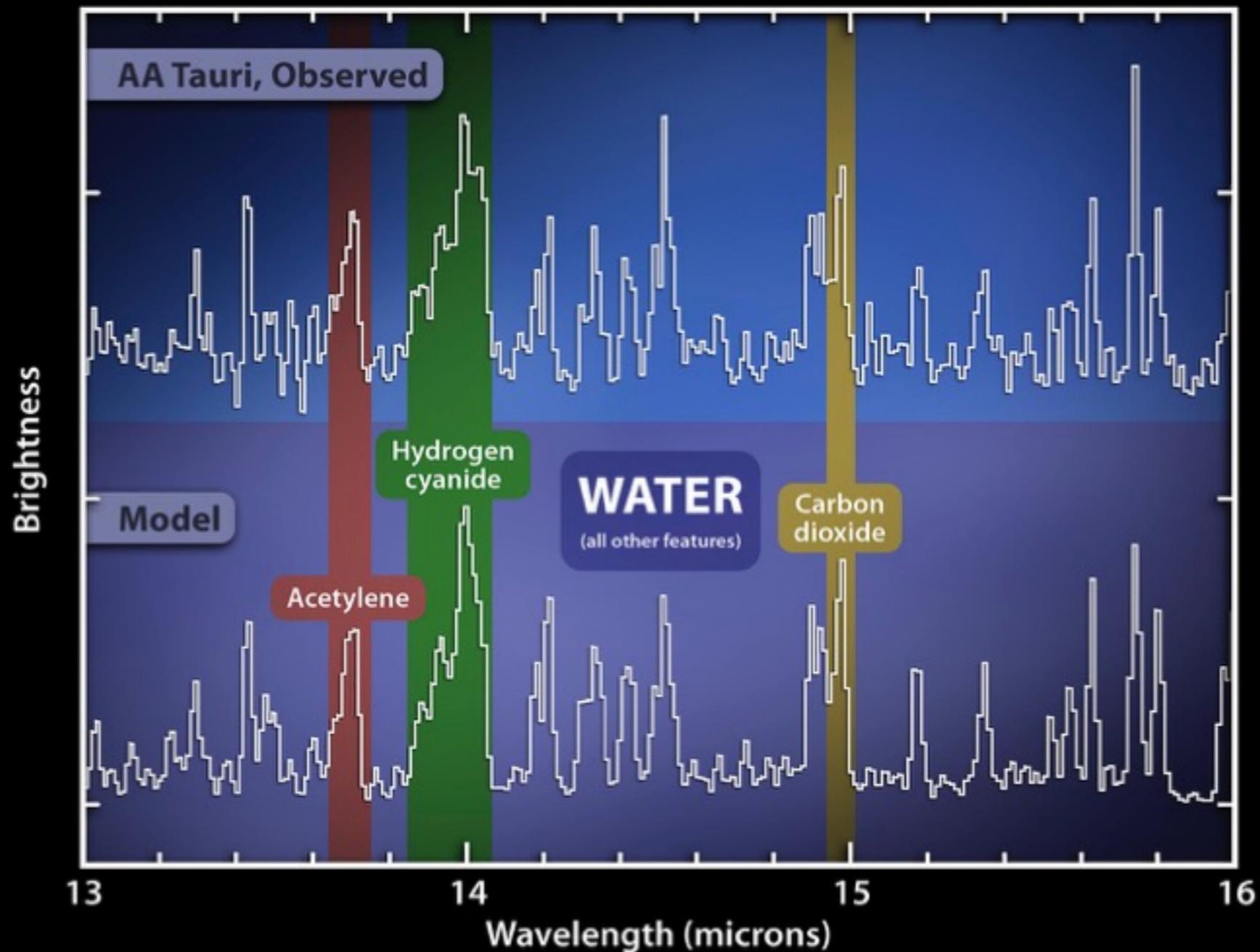


## Ion-molecule Chemistry in Ices

- Ices are charged & charges are localized:
  - Na, PAHs
  - $OCN^-$
  - Polarization charge
- Warm-up leads to segregation
- H-bonding
- Stereochemistry
- Methanol drives chemistry
- Near evaporation, “droplets” may conduce methyl transfer without fragmentation

charged ices: Bouwman et al, 2011, A&A, 529, 46; Schutte et al, 2003, 398, 1049; Demyk et al, 1998, A&A, 339, 553; Balog et al 2009, Phys Rev Lett, 201, 73003

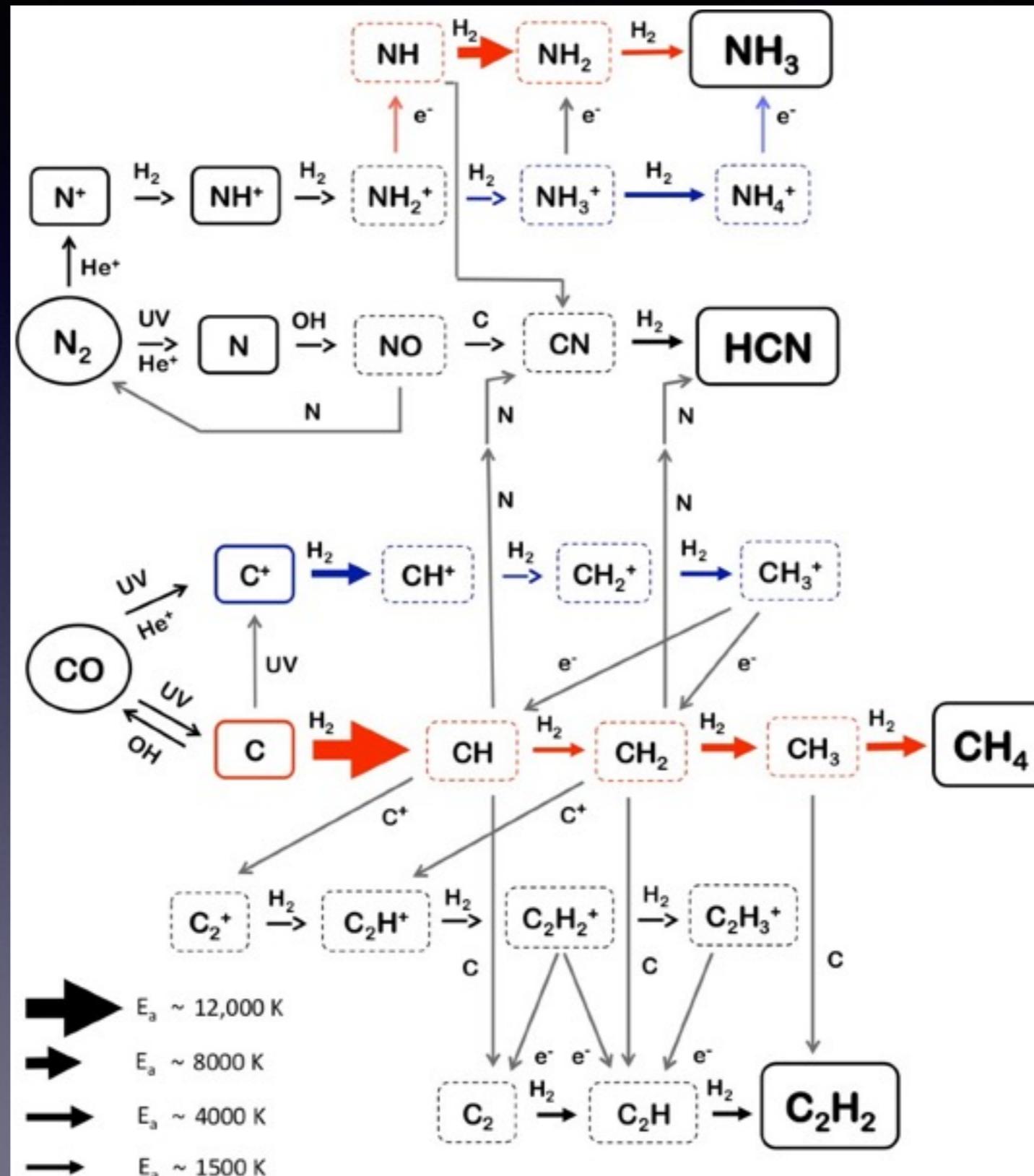
# Warm organics in protoplanetary disks



## Photo-Chemistry in Warm Surface Layers

Najita et al, 2003, ApJ, 589, 931  
Carr & Najita, 2011, ApJ, 733, 102  
Lahuis et al, 2006, ApJ, 636, L145  
Salyk et al, 2011, ApJ, 731, 130

# Chemistry in warm, UV/X-ray irradiated gas



# Building the Solar System's Organic Inventory

From small to big



Protective environment of dense clouds

From big to small



Stars as sooting candles

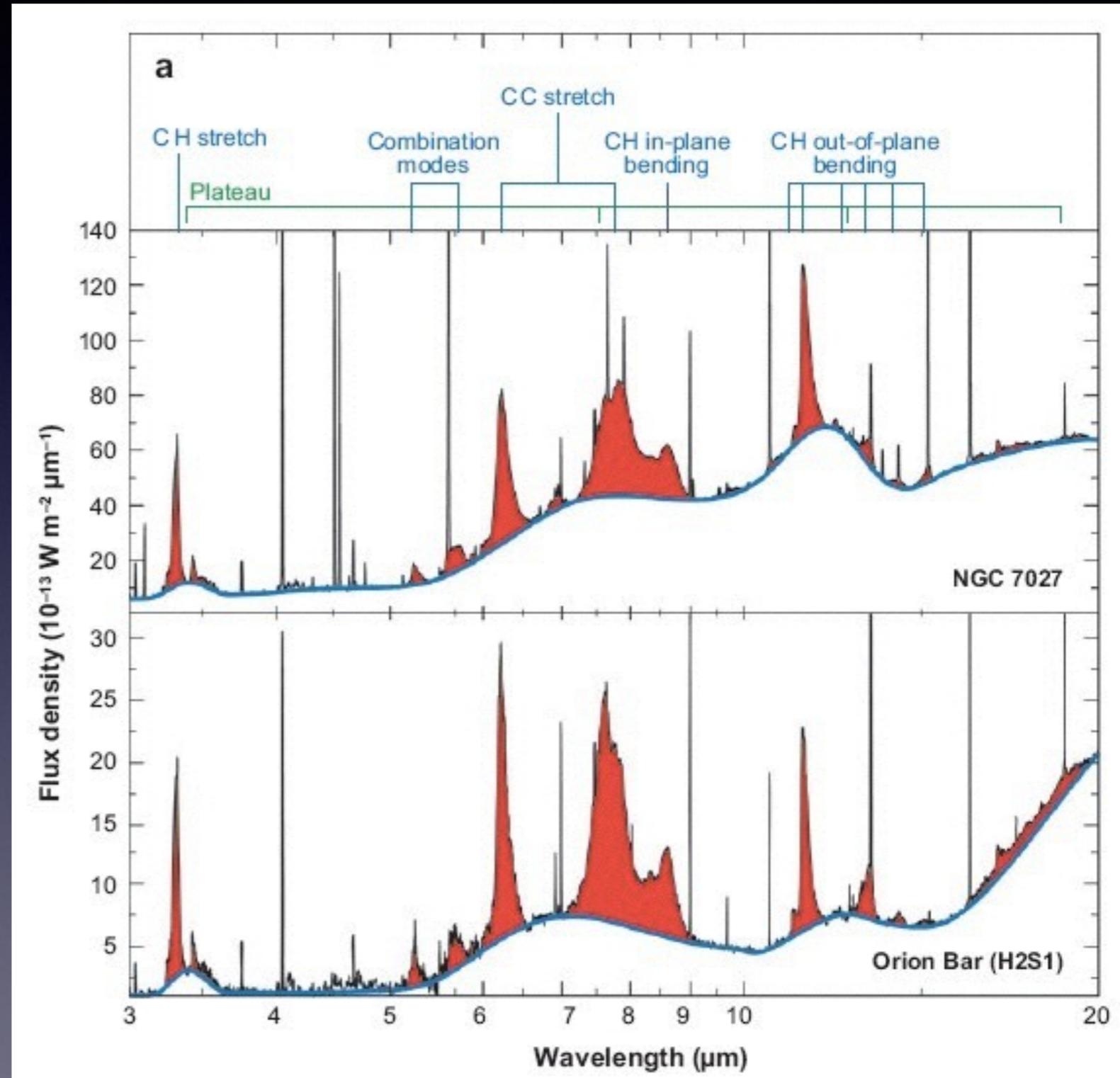
Comets

Asteroids

Chemical growth: a few atoms at a time

UV and energetic particle processing

# The incredibly rich spectrum of interstellar PAHs



# Orion



# PAHs in Orion



Visible

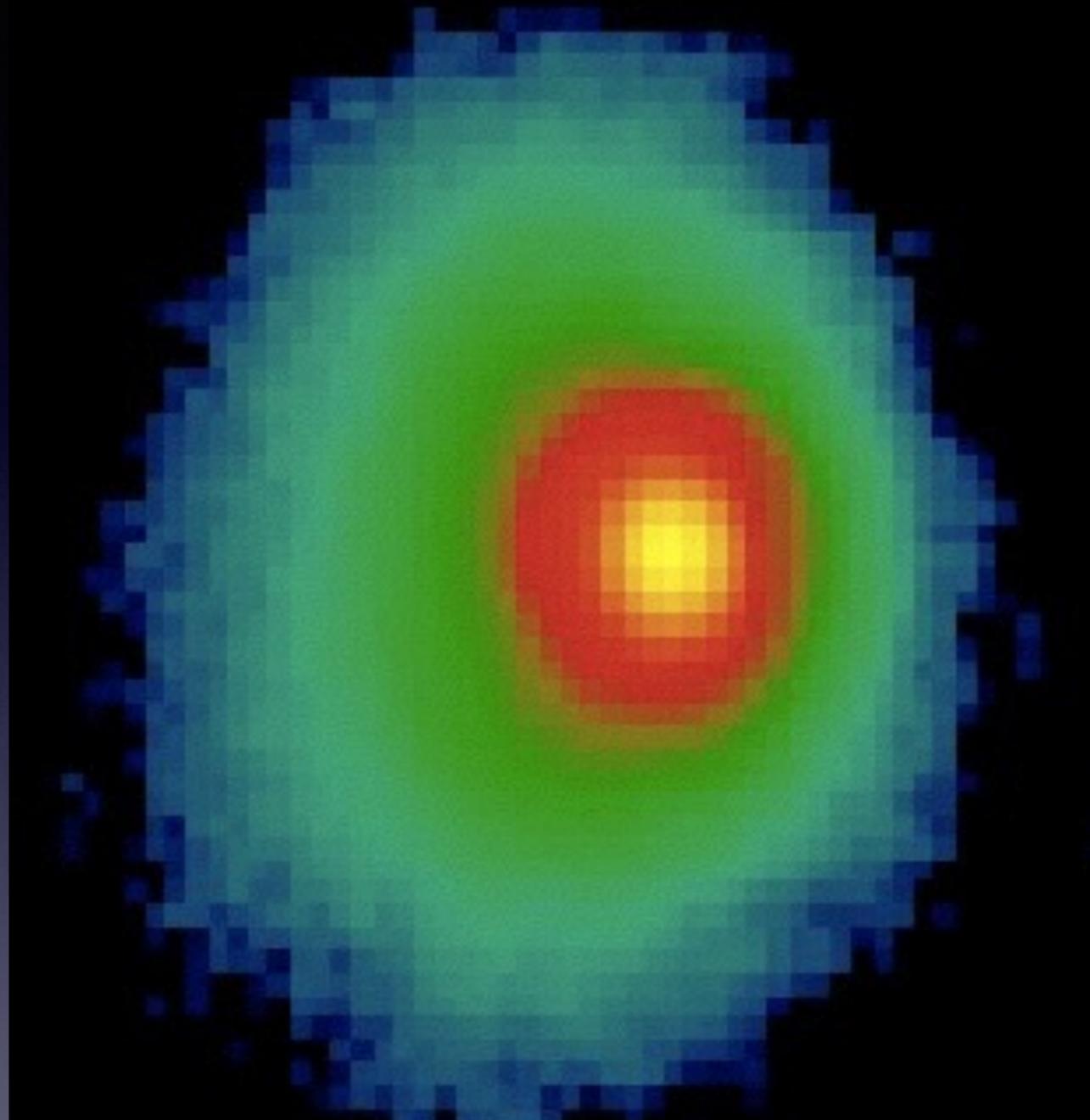


M51: The Whirlpool Galaxy

Infrared



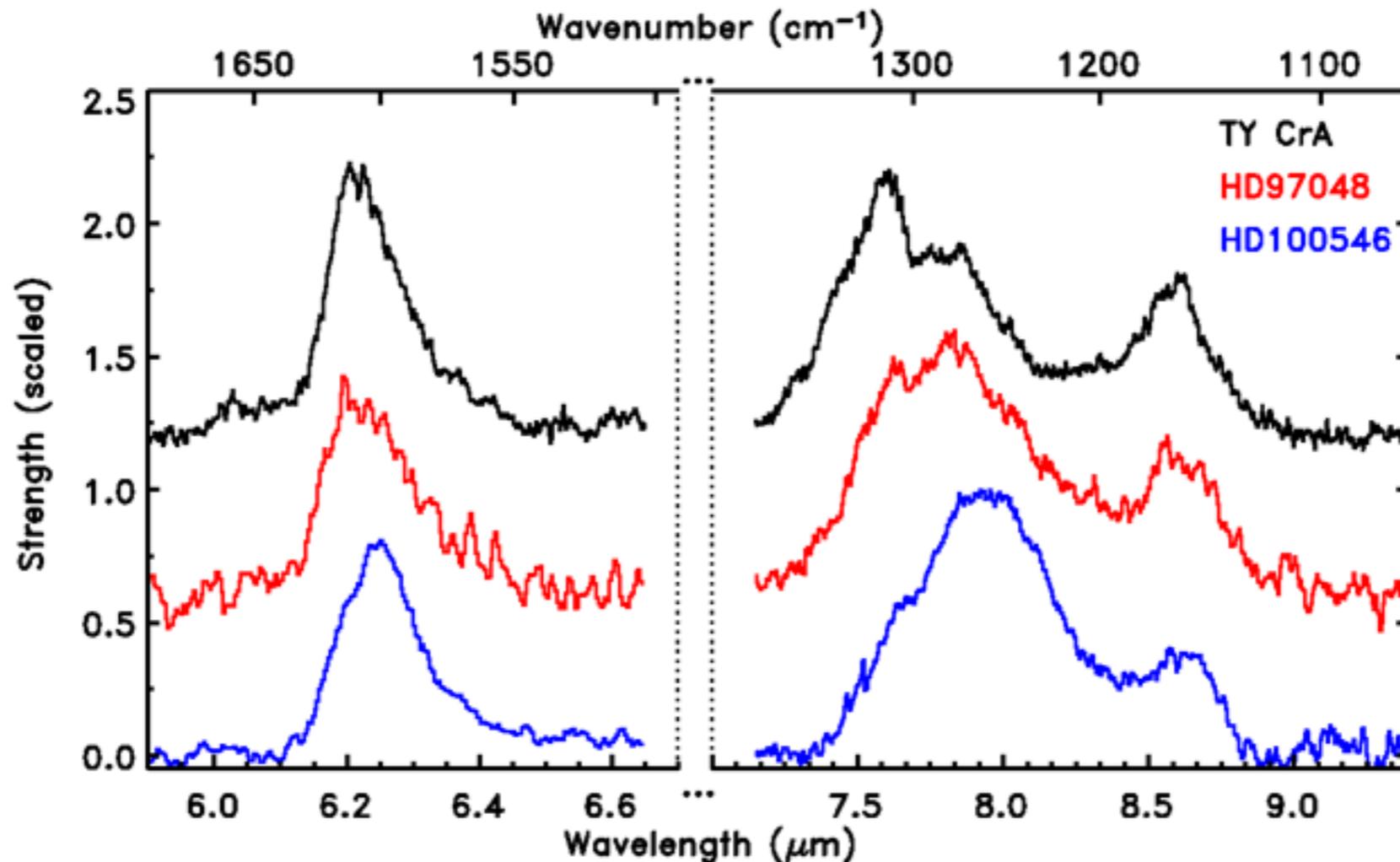
M51: The Whirlpool Galaxy



# PAHs in the Protoplanetary Disk of HD 97048

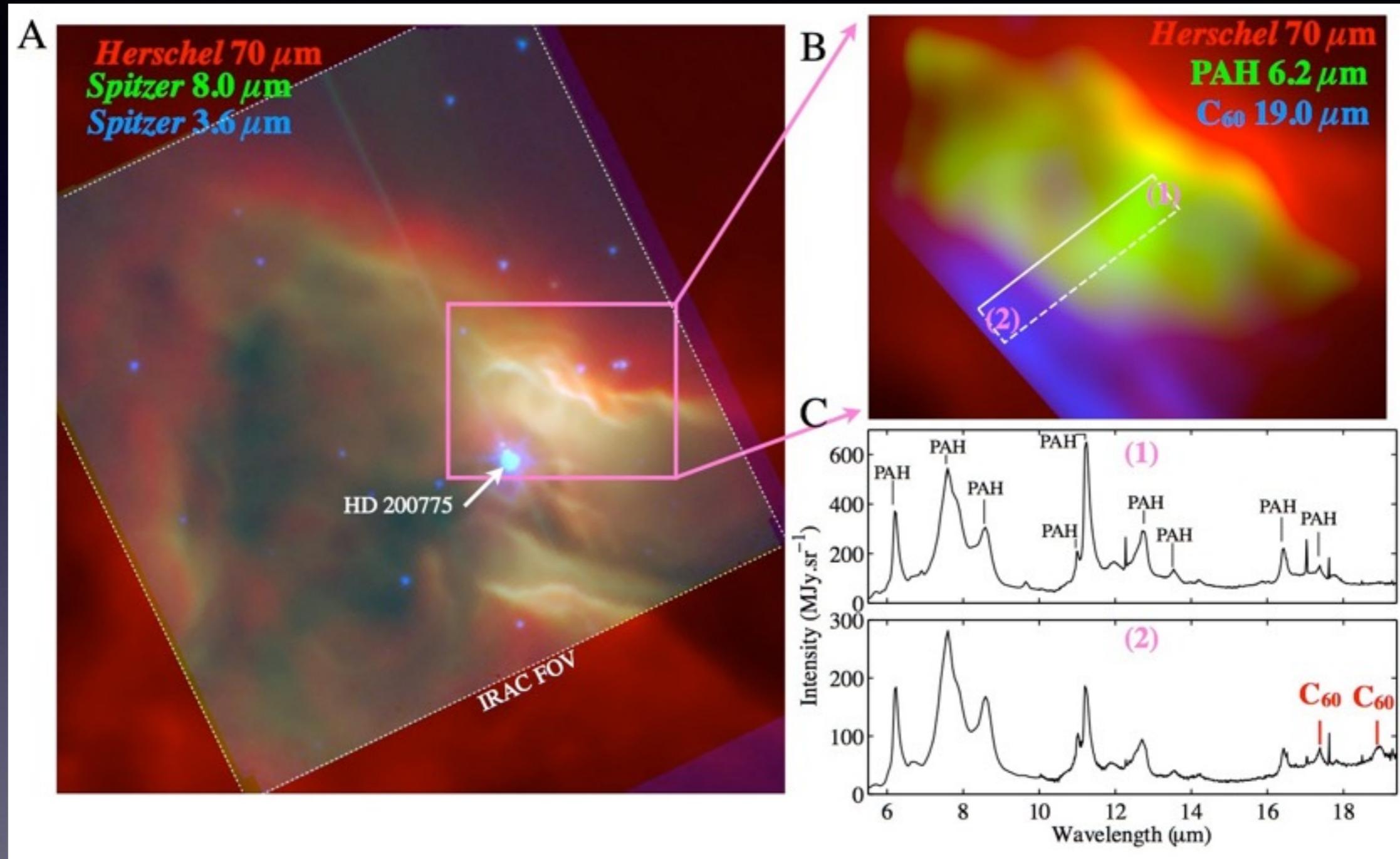
Doucet et al 2007, A&A, 470, 625

# PAHs and Herbig Stars

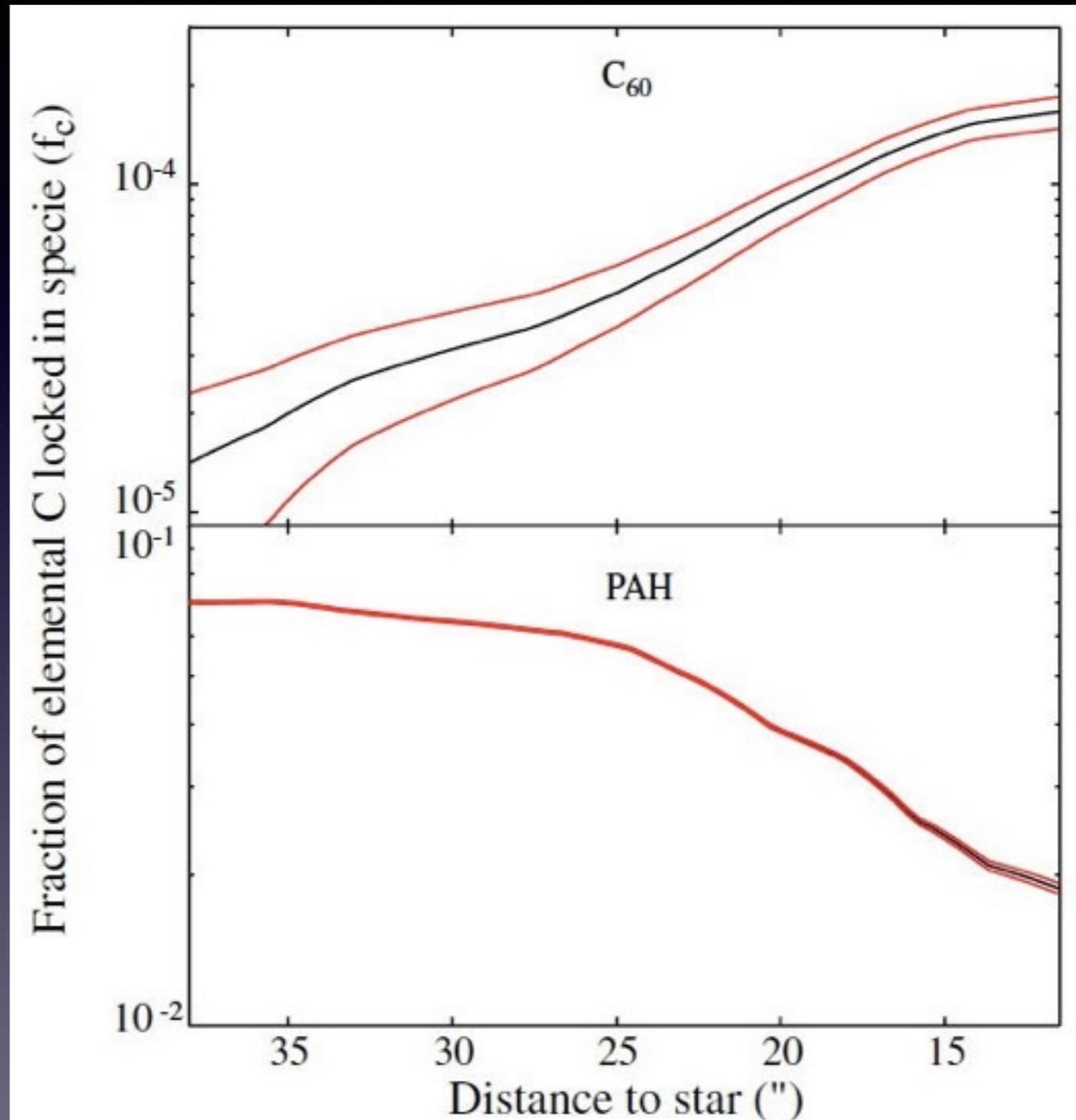


Source	Sp T	Size	Location
TY Cra	B7-B9	~2000 AU	HAeBe in cloud
HD 97048	B9-A0	~100-1000 AU	HAeBe cloud edge
HD 100546	B9	~150 AU	isolated HAeBe star

# PAHs & C<sub>60</sub> in NGC 7023

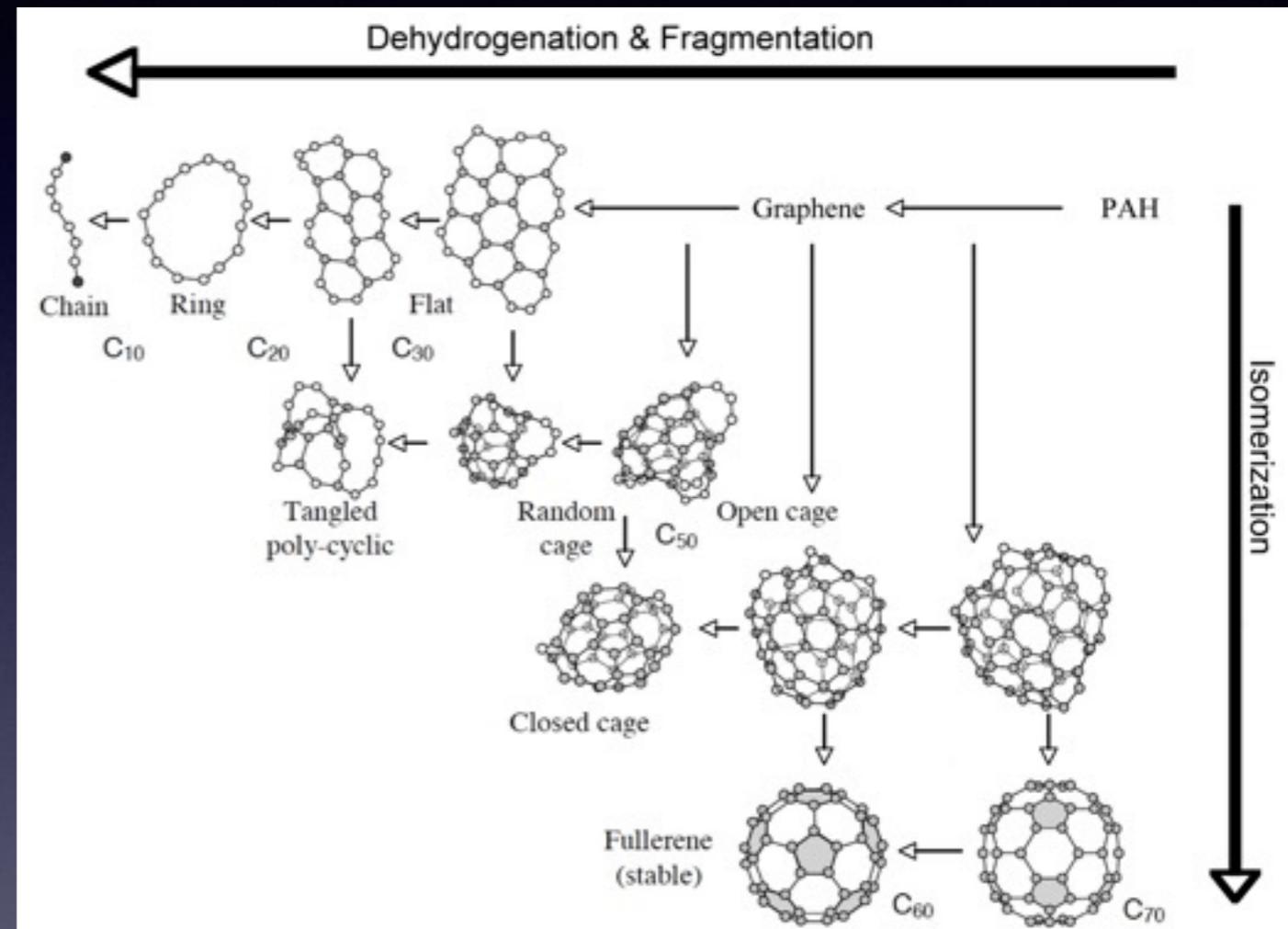


# PAHs & C<sub>60</sub> abundance



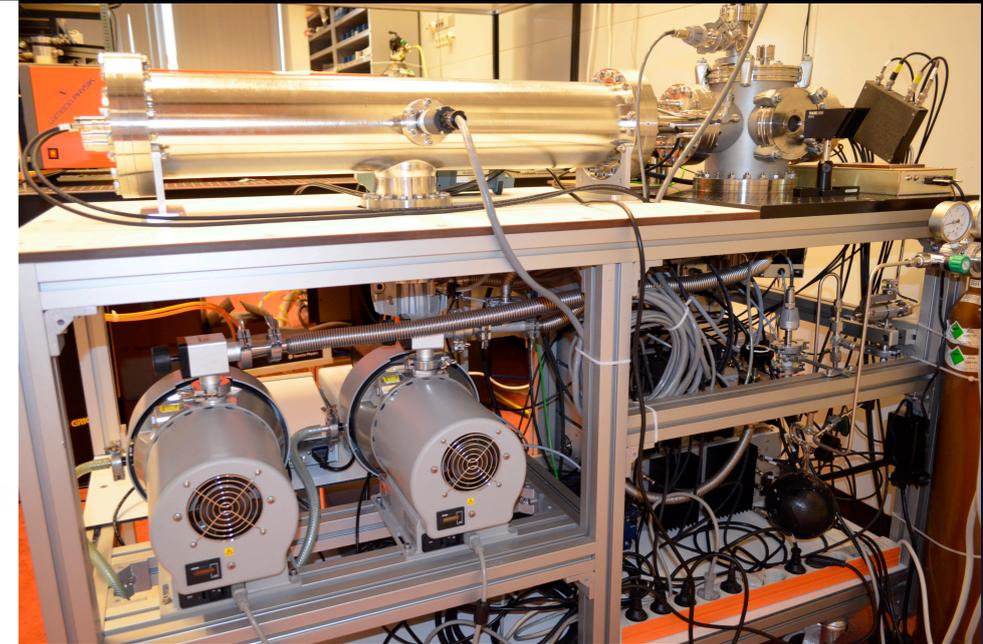
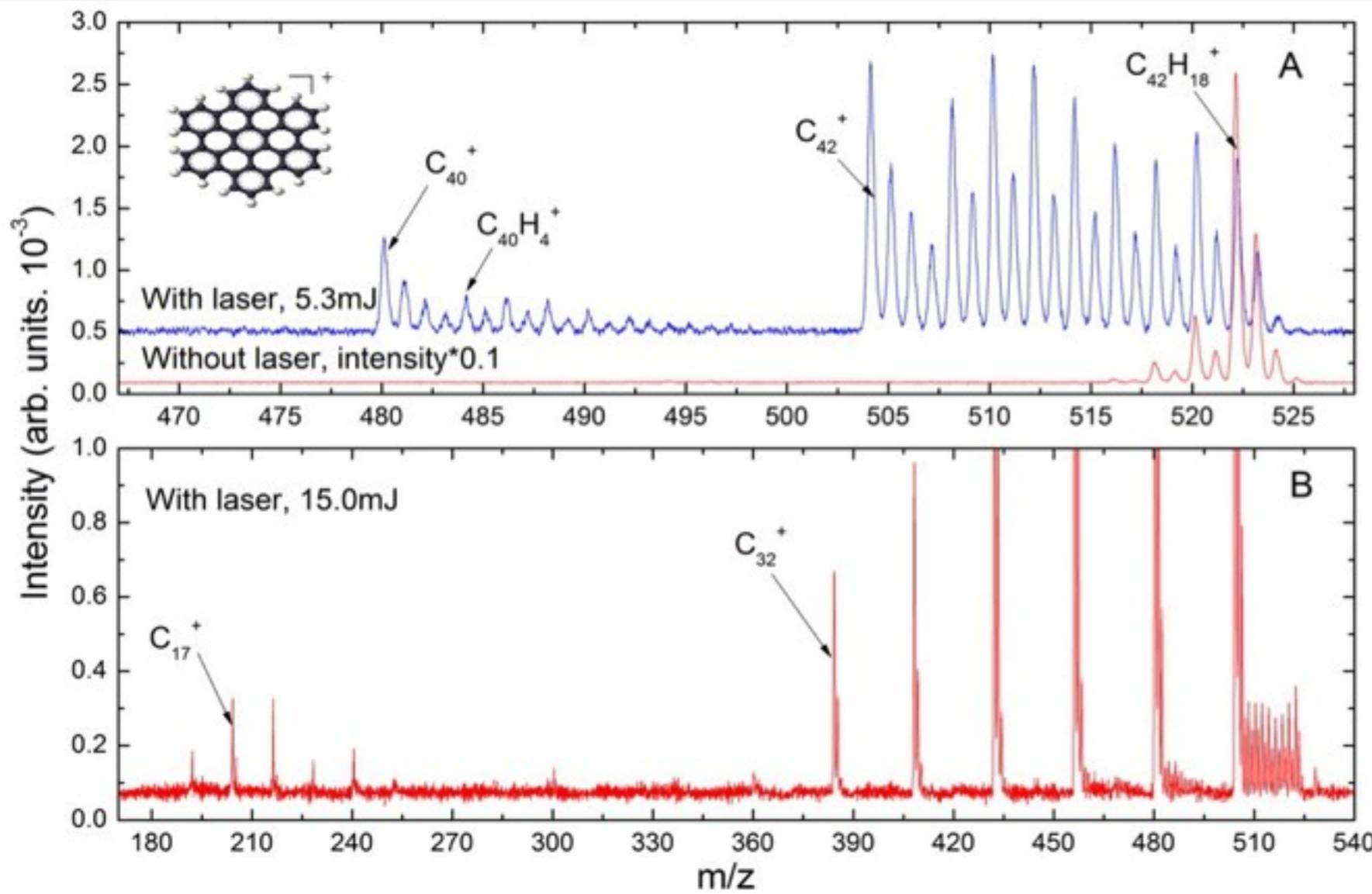
# PAH photolysis

- Dehydrogenation & isomerization
- Stable intermediaries: cages & fullerenes
- Fragmentation products: hydrocarbon chains & radicals



Berne & Tielens, 2012, PNAS, 109, 401  
Pety et al, 2005, A&A, 435, 885  
Wehres et al, 2010, A&A, 518, 36

# PAHs Photolysis

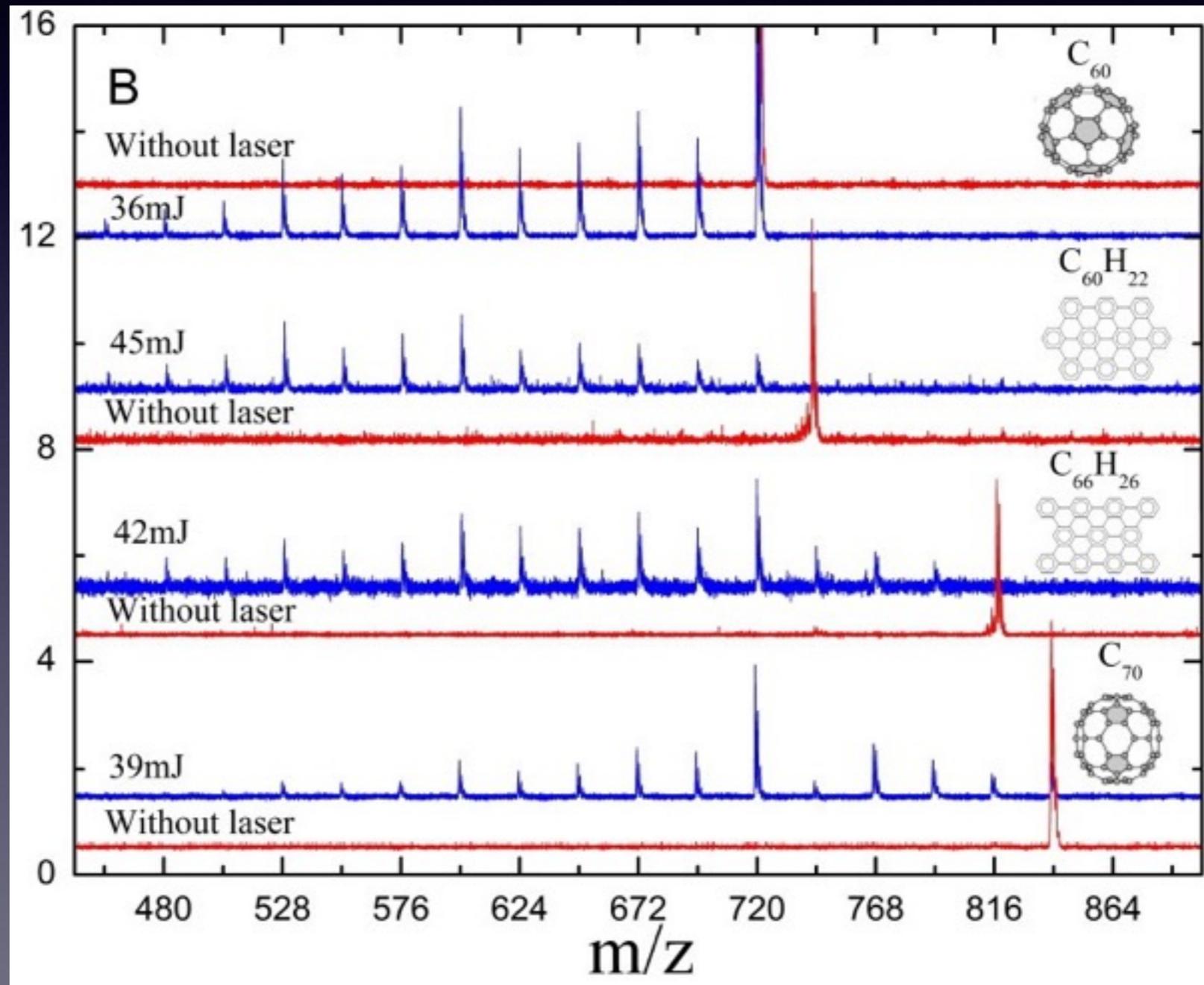


Ekern et al, 1997, ApJ, 488 L39  
Joblin et al, 2003, Edp. Sci. Conf. Ser. 175  
Zhen et al, 2014, Chem Phys Lett, 592, 211

- Multiphoton absorption leads to fragmentation in a laser pulse
- Many pulses strip the molecule down
- Loss of all H followed by loss of  $C_2$  and C units (magic numbers)

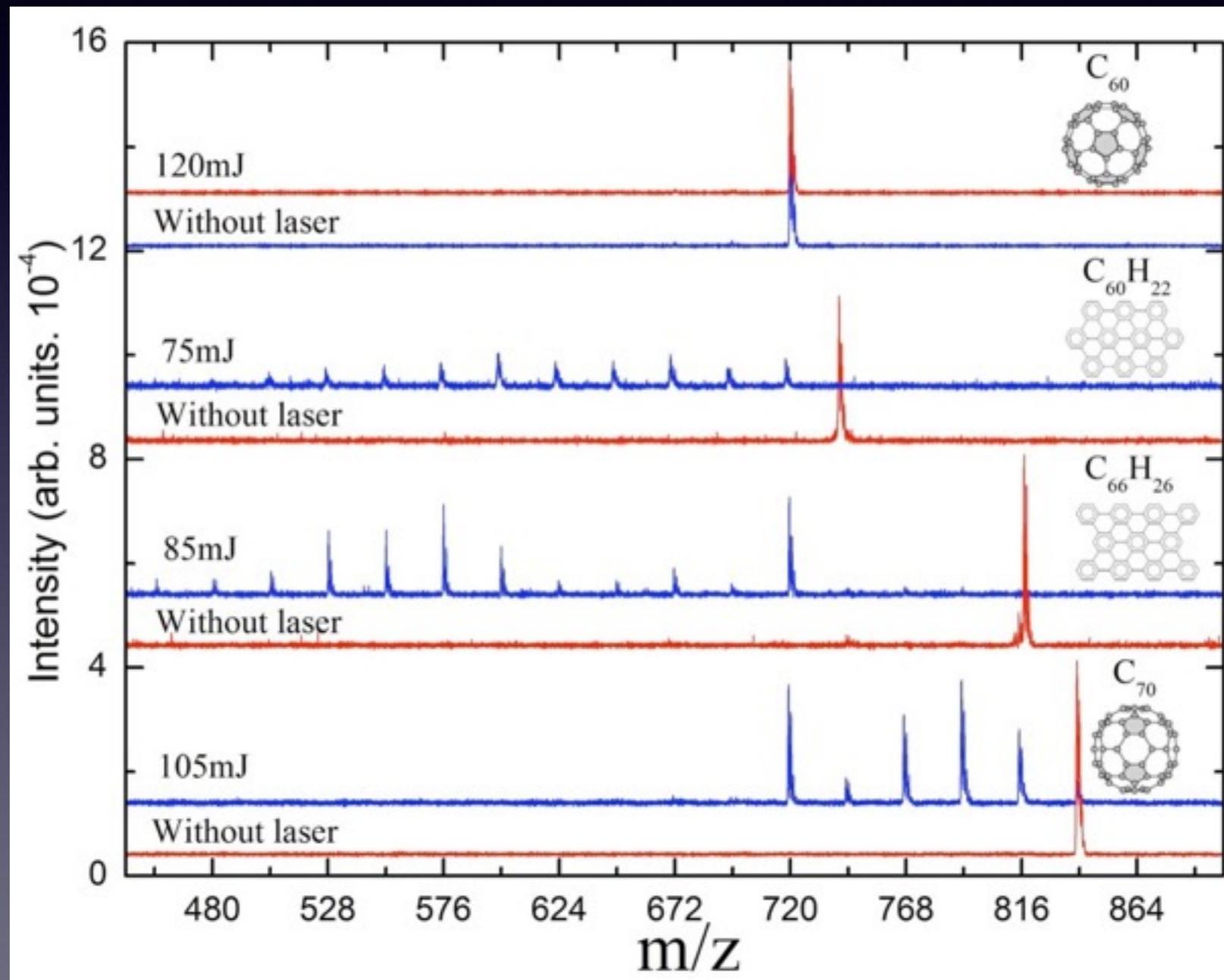
# From PAHs to C<sub>60</sub>

UV photolysis at 355 nm



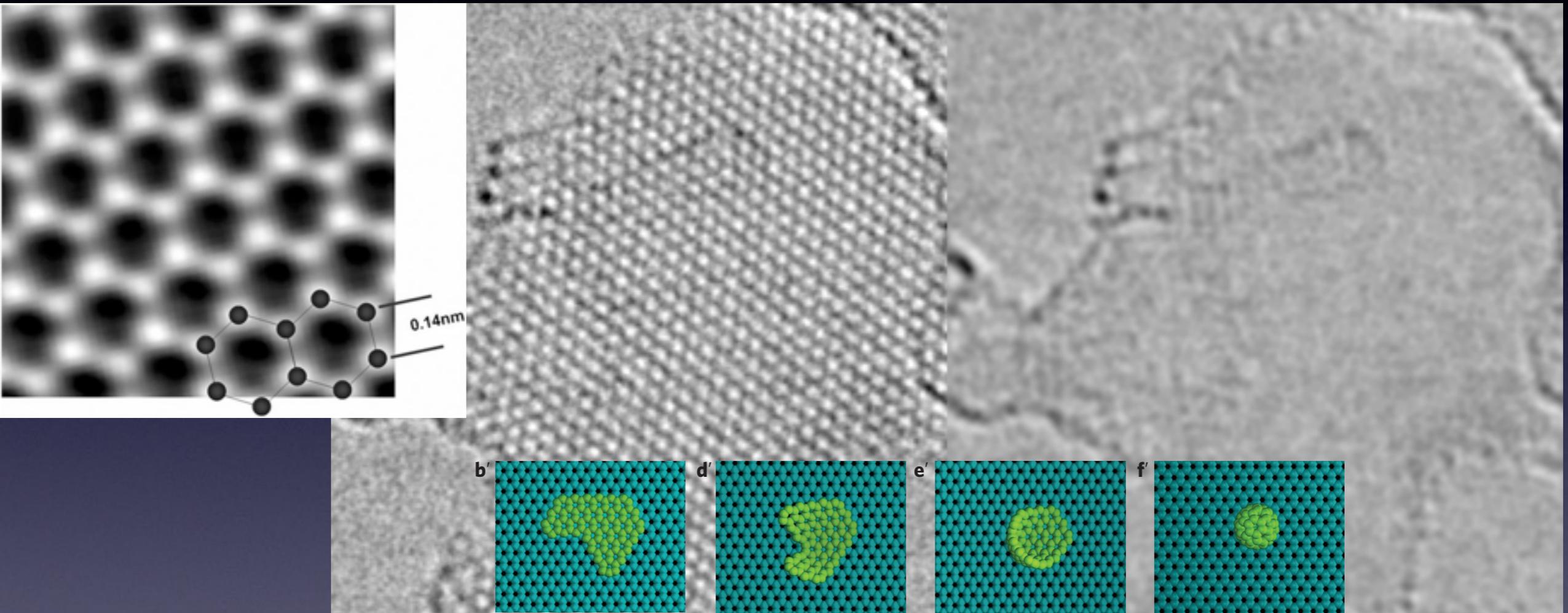
# From PAHs to C<sub>60</sub>

UV photolysis at 532 nm



# From Graphene to C<sub>60</sub>

[National Center for electron microscopy]



[Chuvilin et al. Nature Chem. 2010]

Transformation of graphene to C<sub>60</sub>, driven by electron irradiation



Imagine Brazil as Soccer Champions  
of the molecular Universe !!

# The Organic Inventory of Comets

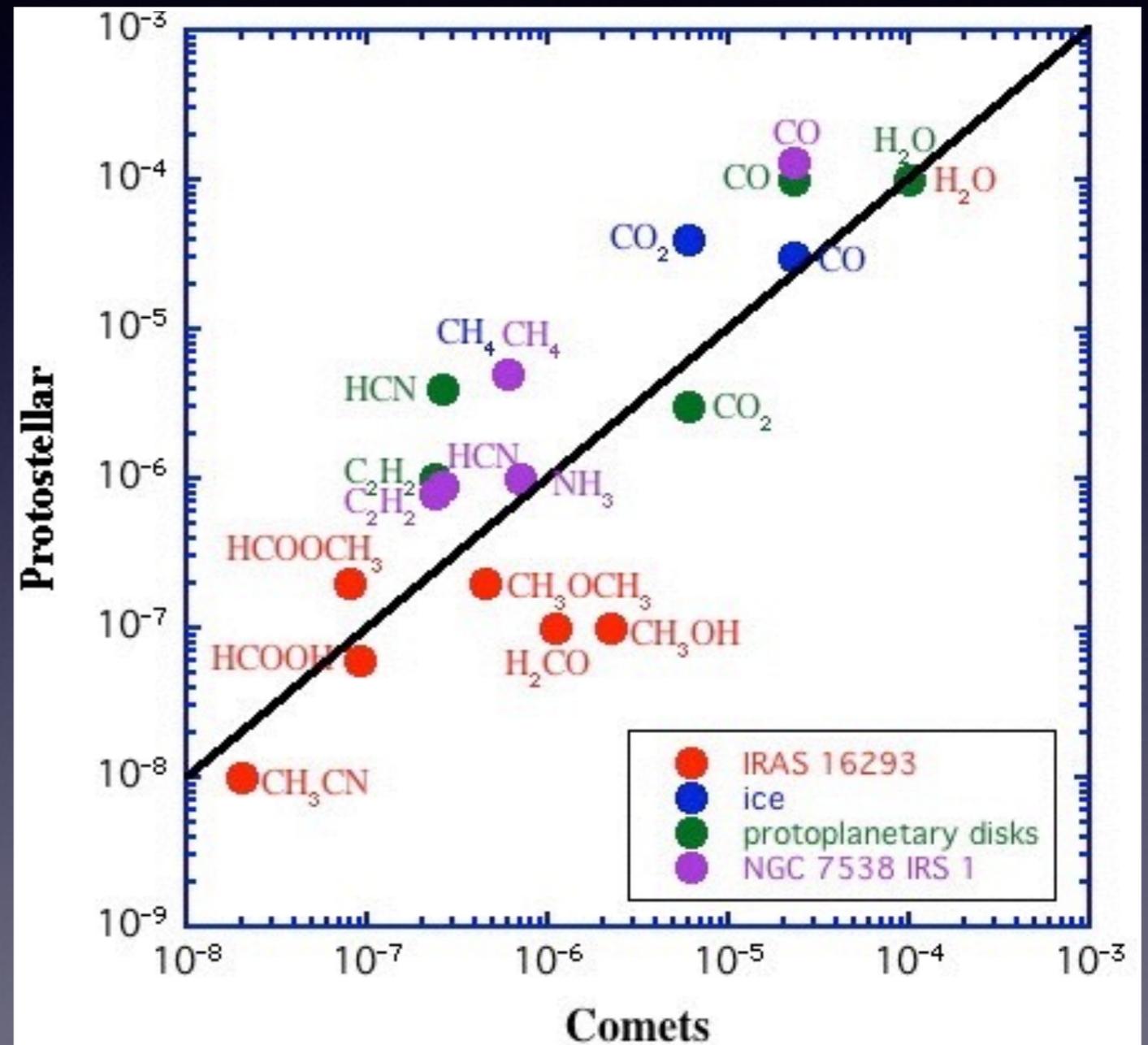
Comets, and hence the Earth, sampled many reservoirs with a diverse chemical history

ice chemistry

Hot Core chemistry

Warm gas photochemistry

PAHs



# Key Questions

- Building new worlds: What are the key processes in planet formation ? How do they depend on the environment ? What is the inventory of planets, particularly in the habitable zone ?
- Planetary habitats: What are the primordial sources of organics and volatiles and the processes that play a role in their formation and delivery ?
- Setting the stage for life: What are the conditions on the early Earth & newly formed planets and what are the key processes that set the stage for life ?

# Future of Astrochemistry

- Paradigms have been developed which provide precise descriptions of the various stages in the formation and early evolution of planetary systems
- Goal for the near future:
  - Review these paradigms & determine how accurate are
  - Predict the composition of terrestrial exoplanets & exomoons
  - Predict biosignatures of exoplanets

Kepler, TESS & Plato



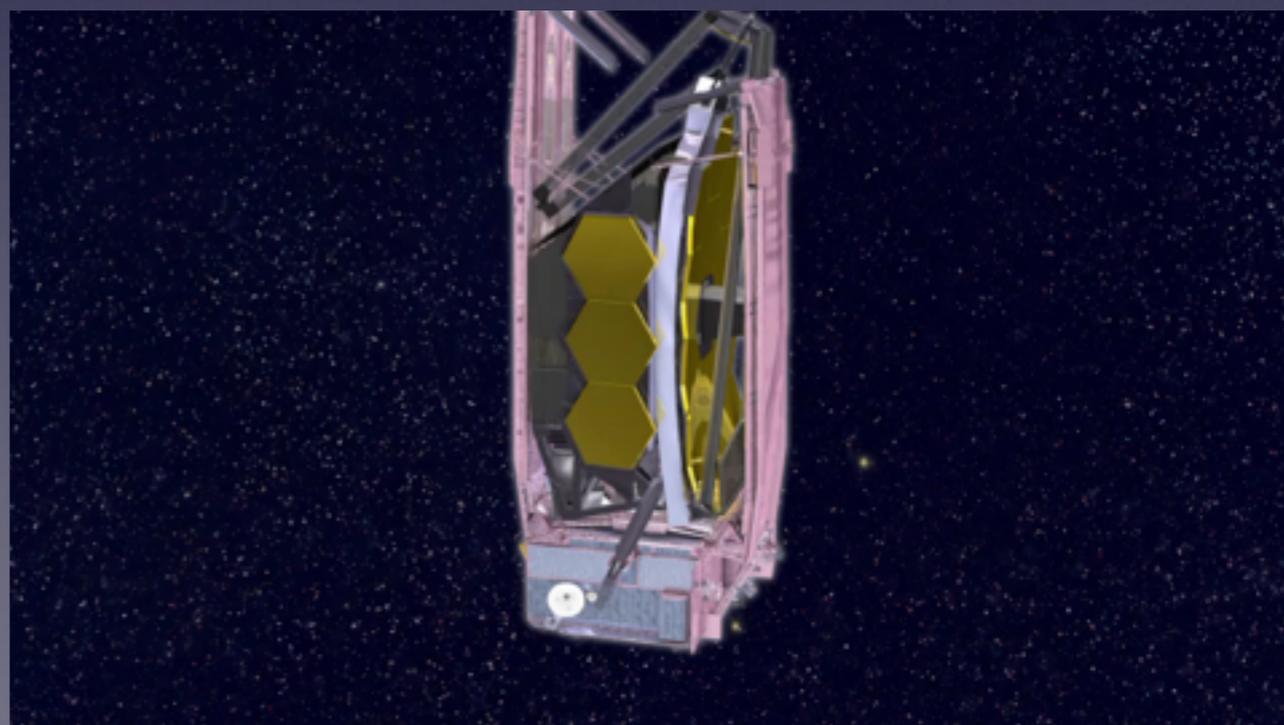
ALMA



SOFIA



James Webb





Cassini/Huygens

Free Fall  
6630 km  
20013 km/h  
8:50 UT



esa

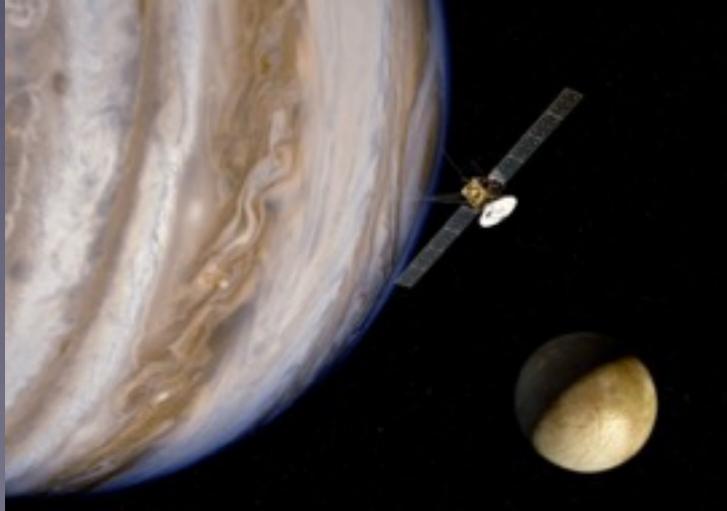
Rosetta visits Lutetia

Rosetta



Stardust

Curiosity



Juice

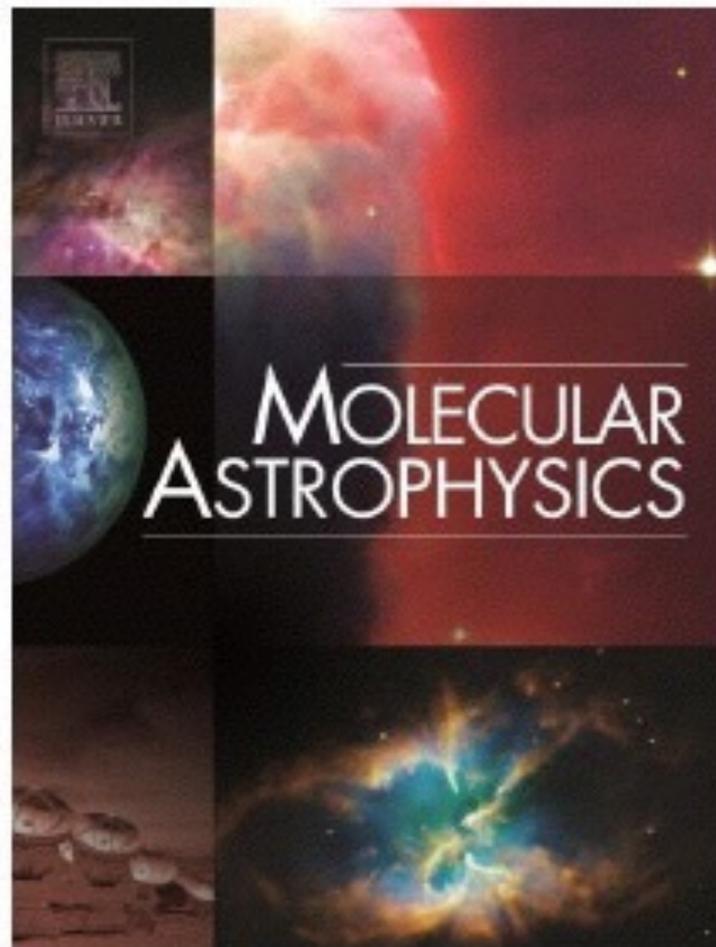


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