Hydrogen cyanide and the computational origin of life

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Hydrogen cyanide and the computational origin of life

Goal:

to understand possible prebiotic chemical systems using both laboratory experiments (**Martin**) and computer modeling (**Daniel**)

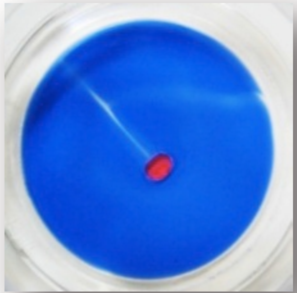
Hydrogen cyanide and the computational origin of life

Part 1:

Introduction to self-moving chemical systems

Self-moving systems and the origin of life

Introduction to self-moving chemical systems

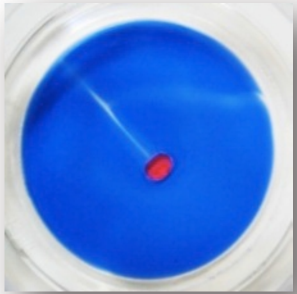


Droplets

- Self-moving and chemotactic

Goal: create an instability-driven, self-moving artificial system

Introduction to self-moving chemical systems



Droplets

- Self-moving and chemotactic

Oil: nitrobenzene (heavy and non-reactive)

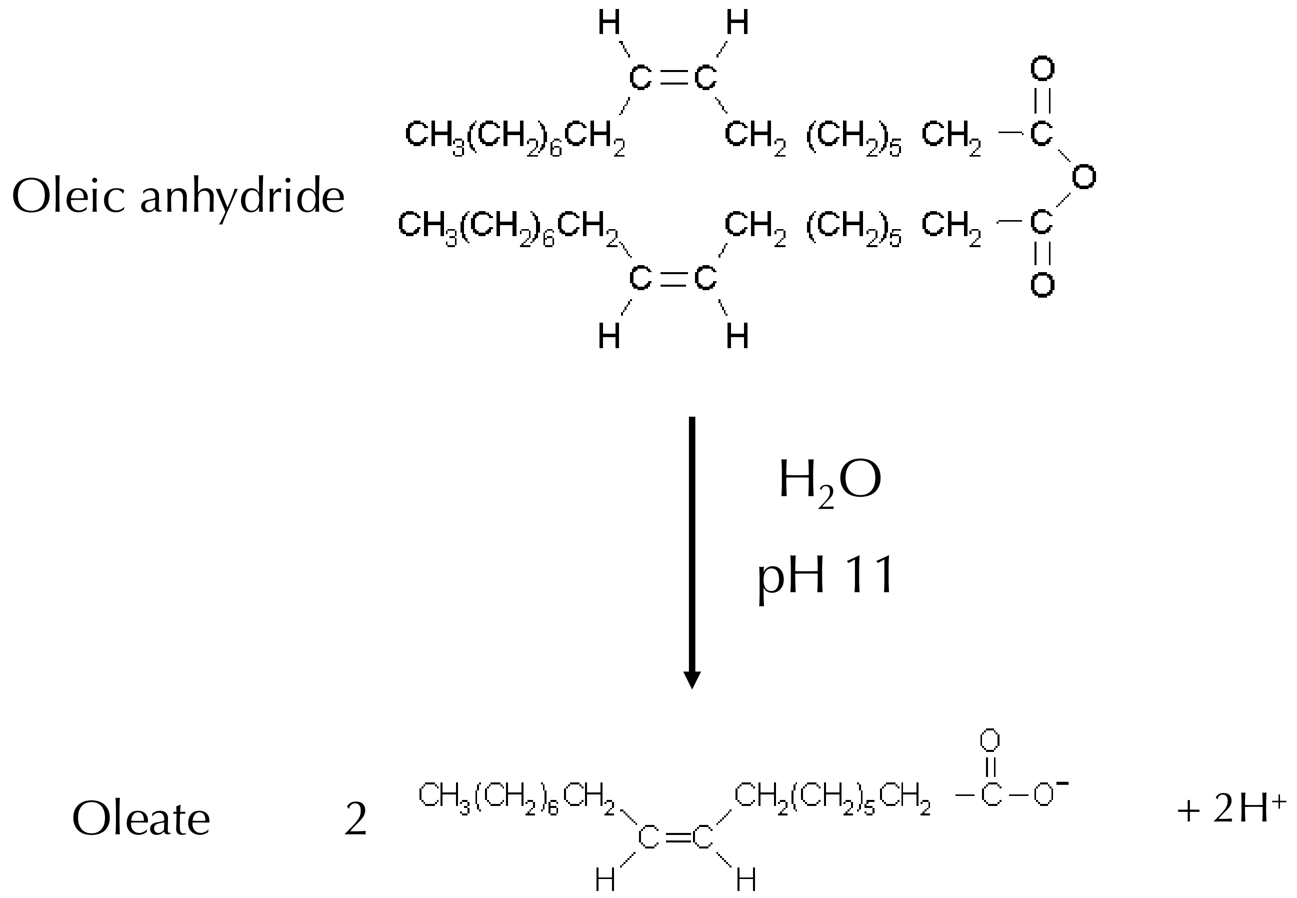
Fuel: oleic anhydride

Reaction: anhydride hydrolysis

Environment: water

Space: glass dish

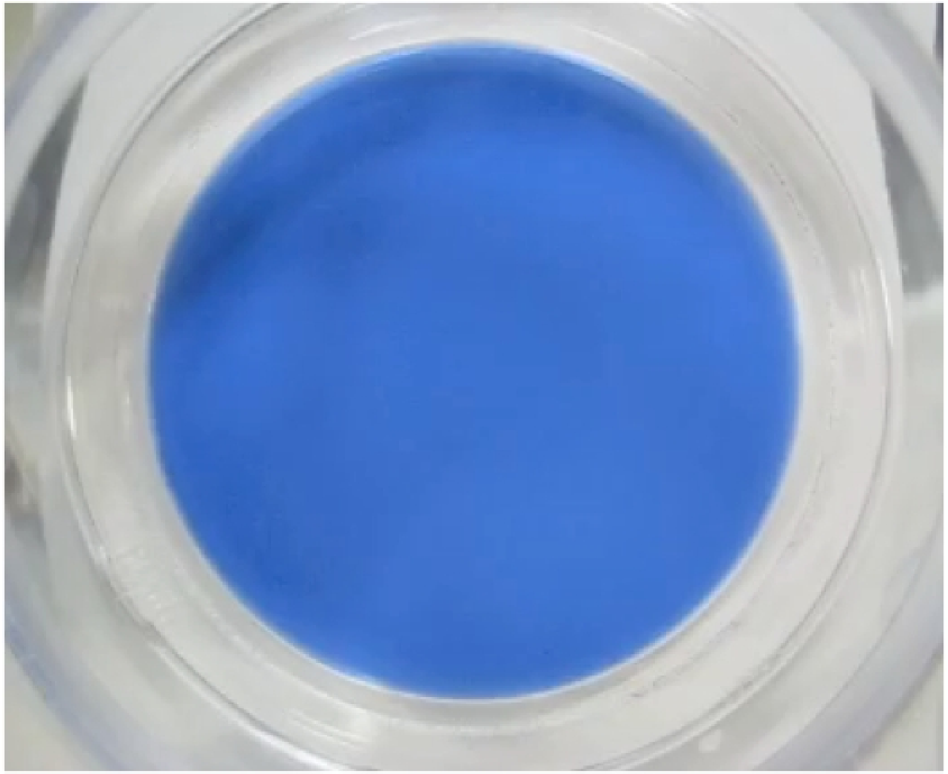
Droplet: internal 'metabolism'



Chemistry from: Autopoietic Self-Reproduction of Fatty Acid Vesicles. Walde, Wick, Fresta, Mangone, Luisi *J. Am. Chem. SOC. 1994,116,* 11649-11654

Droplet:
Self-movement and pH gradients

8X real time movie
5ul nitrobenzene and oleic anhydride droplet 1:1
0.8mL water pH 12.0
0.1mg/ml pH indicator Thymolphthalein



Reference:

pH 12

< pH 11

1cm

pH 9.3-11.5 transition from blue to colorless solution

Hanczyc MM, et al. 2007. *JACS* 129(30):9386-91.

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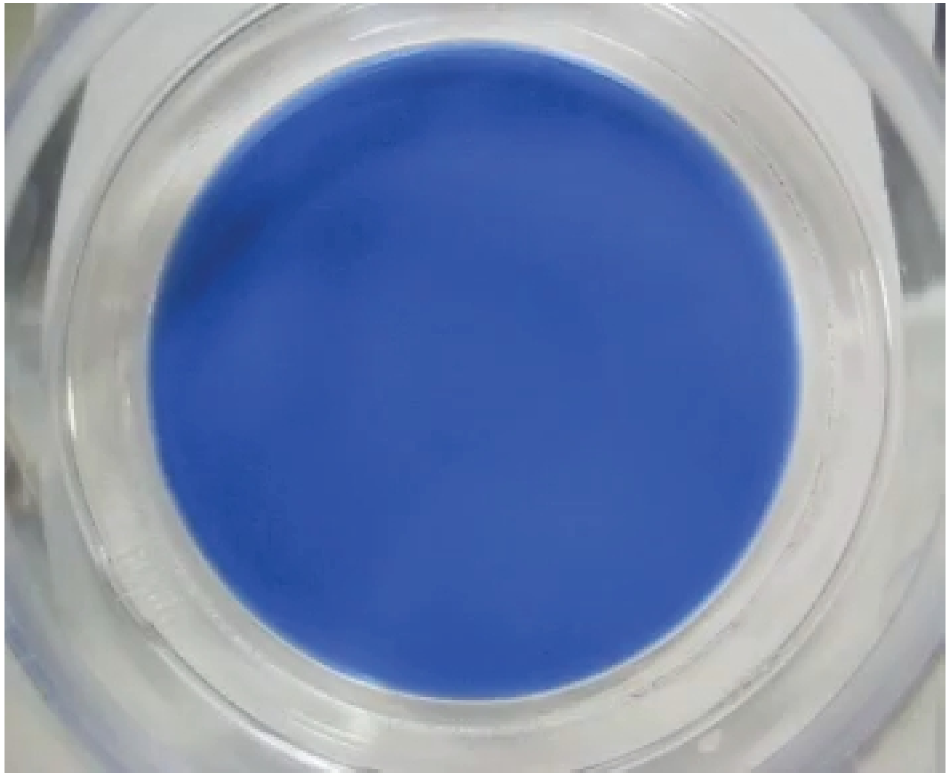
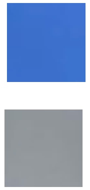


Reference:



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pH 9.3-11.5 transition from blue to colorless solution

https://www.youtube.com/watch?v=DIAQMe2wKZE

Droplet Chemotaxis….

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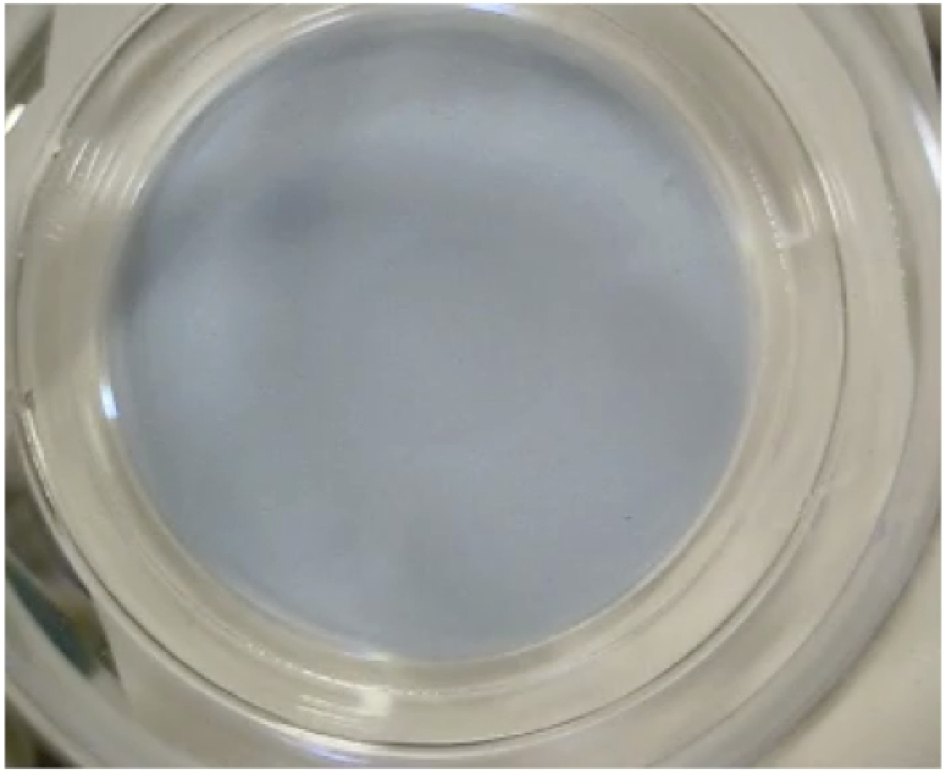
0.1ul 3M NaOH gradient



1cm

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Hanczyc MM, et al. 2007. *JACS* 129(30):9386-91.

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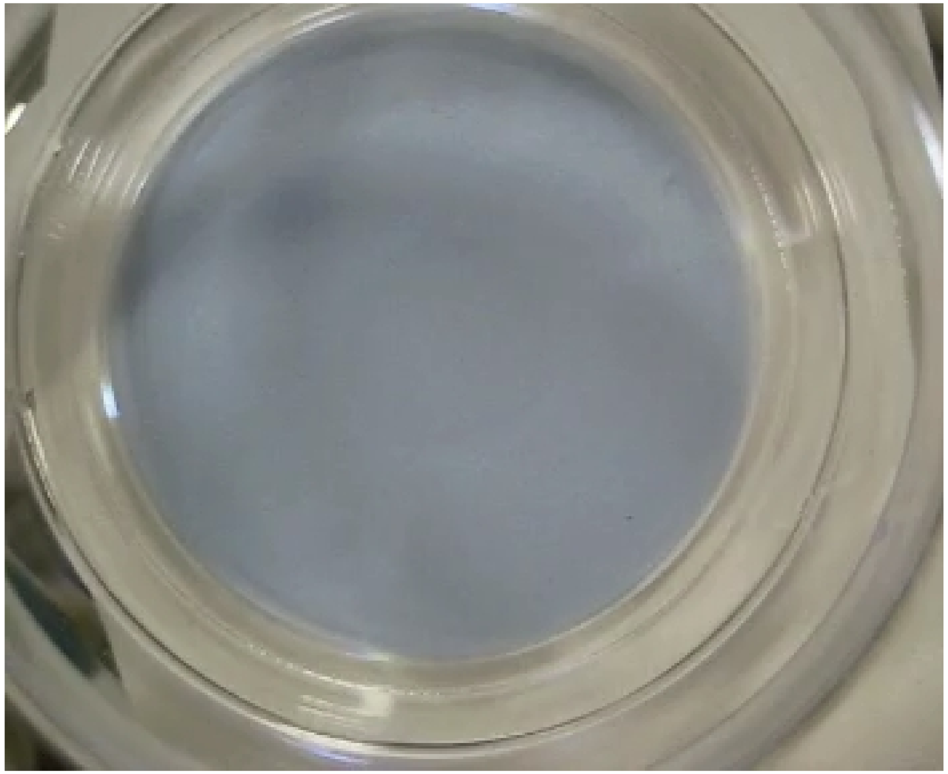


1cm

pH 9.3-11.5 transition from clear to blue solution

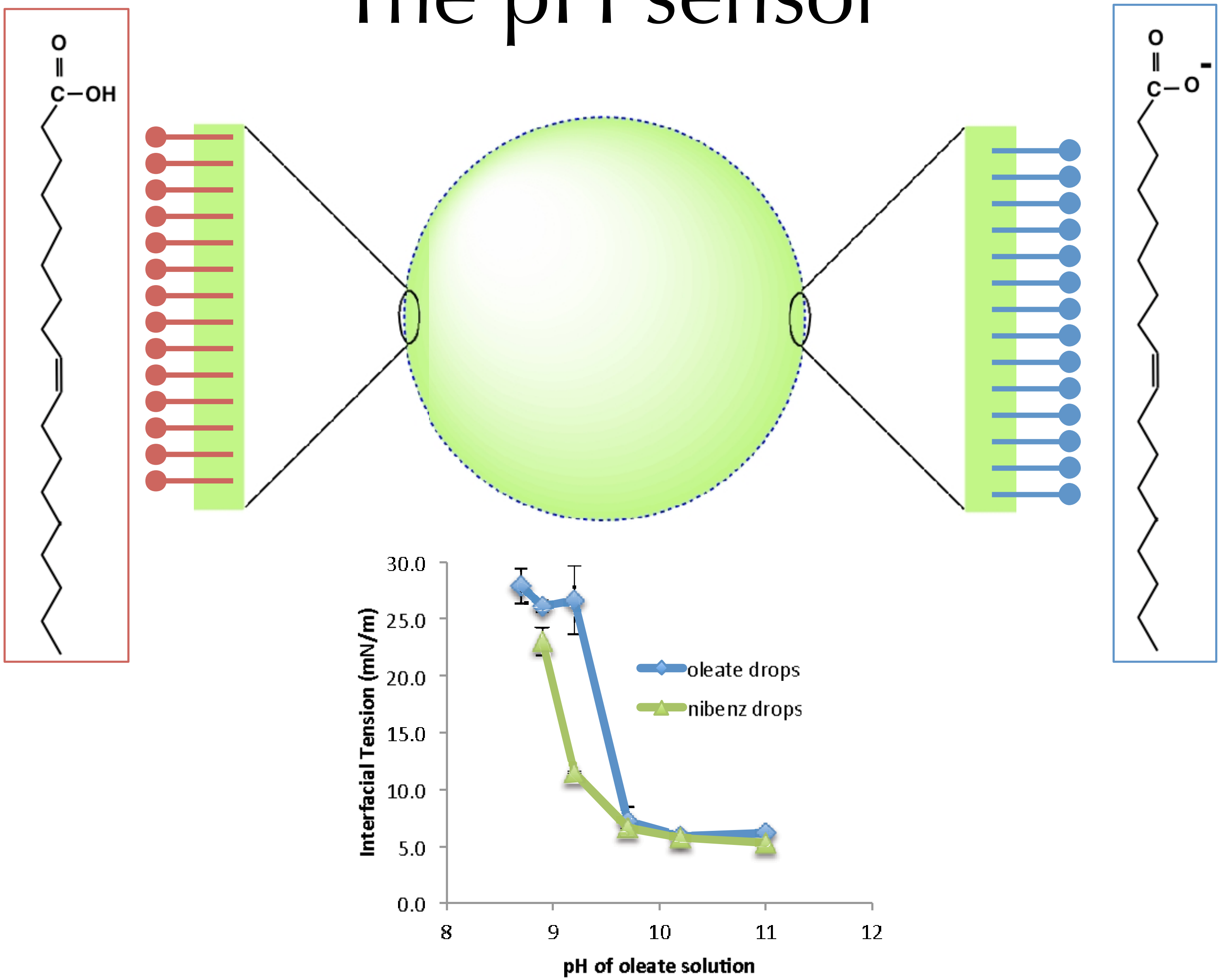
http://www.youtube.com/watch?v=bikzGbcYj10

Reference:

> pH 12

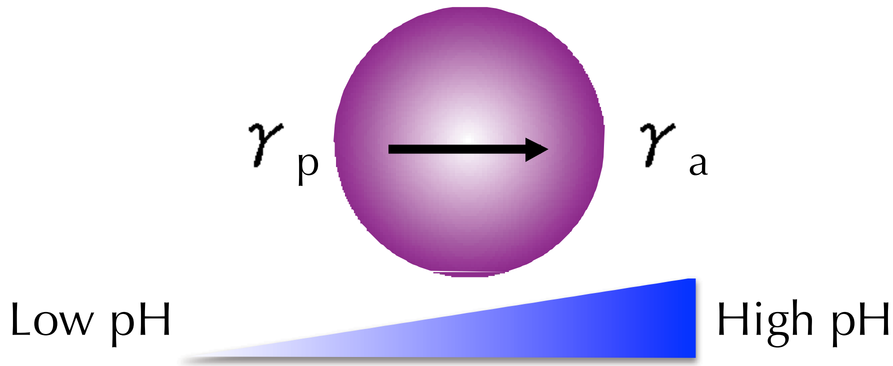
pH 11

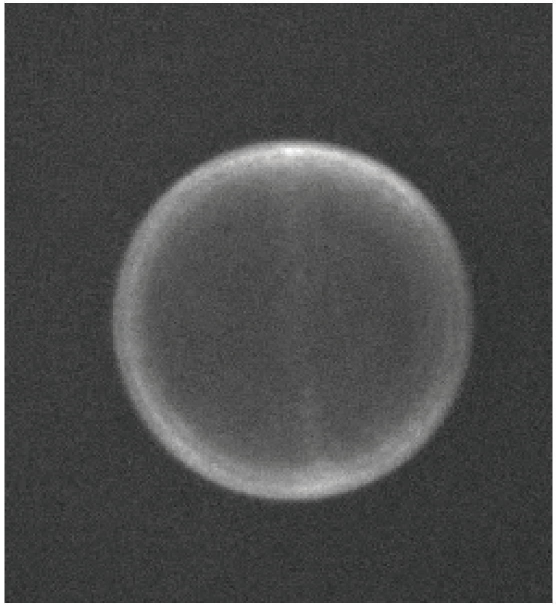
The pH sensor



Droplet motor

Change in pH results in change in interfacial tension which drives convective flow in spherical droplets





In this condition, $\gamma_p >> \gamma_a$ resulting in a Marangoni instability-induced flow of surfactant and convection

Low Reynolds number: viscosity dominates

https://www.youtube.com/watch?v=WlgOEZS_lWw

Droplet Chemotaxis….

Chemical chemotaxis vs biological chemotaxis

1 mm

Droplets exposed to NaOH from a micropipette

http://youtu.be/axooqr3BFtQ

http://www.hopkinsmedicine.org/cellbio/devreotes/videos.htm

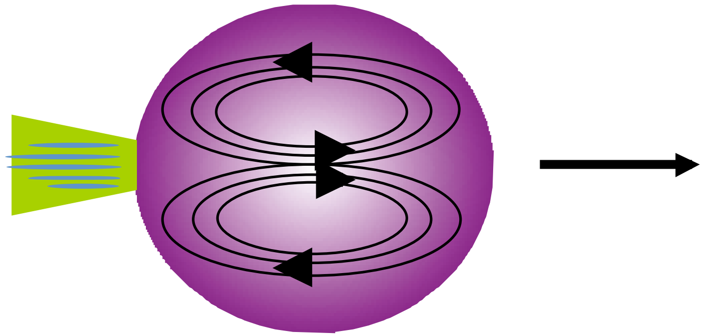
Single Dictyostelium cell exposed to a cyclic AMP gradient from a micropipette. Concentration of cyclic AMP changes ~20% across the cell.

https://www.youtube.com/watch?v=iJBDCMmWr7Q

Introduction to self-moving chemical systems

Self-moving droplets have their own emergent internal mechanism to avoid equilibrium

Not origin of life….



System composition:

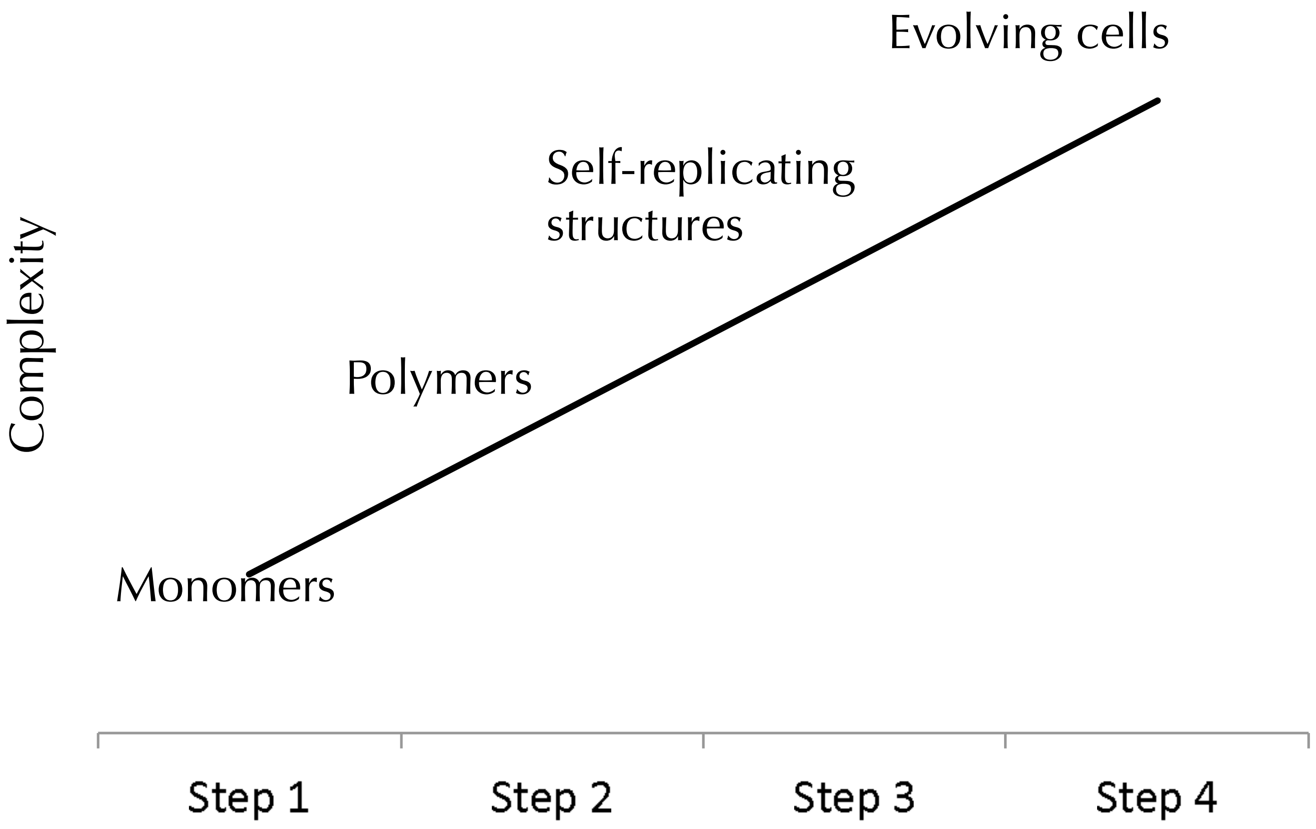
Fuel:	>95% oleic anhydride
Surfactant:	>95% Na-oleate
Oil:	>99% nitrobenzene

Self-moving systems and the origin of life

Uncontrolled chemical reactions produces a diverse mixture of organic compounds: a pool too difficult to fully characterize. The product looks like tar.

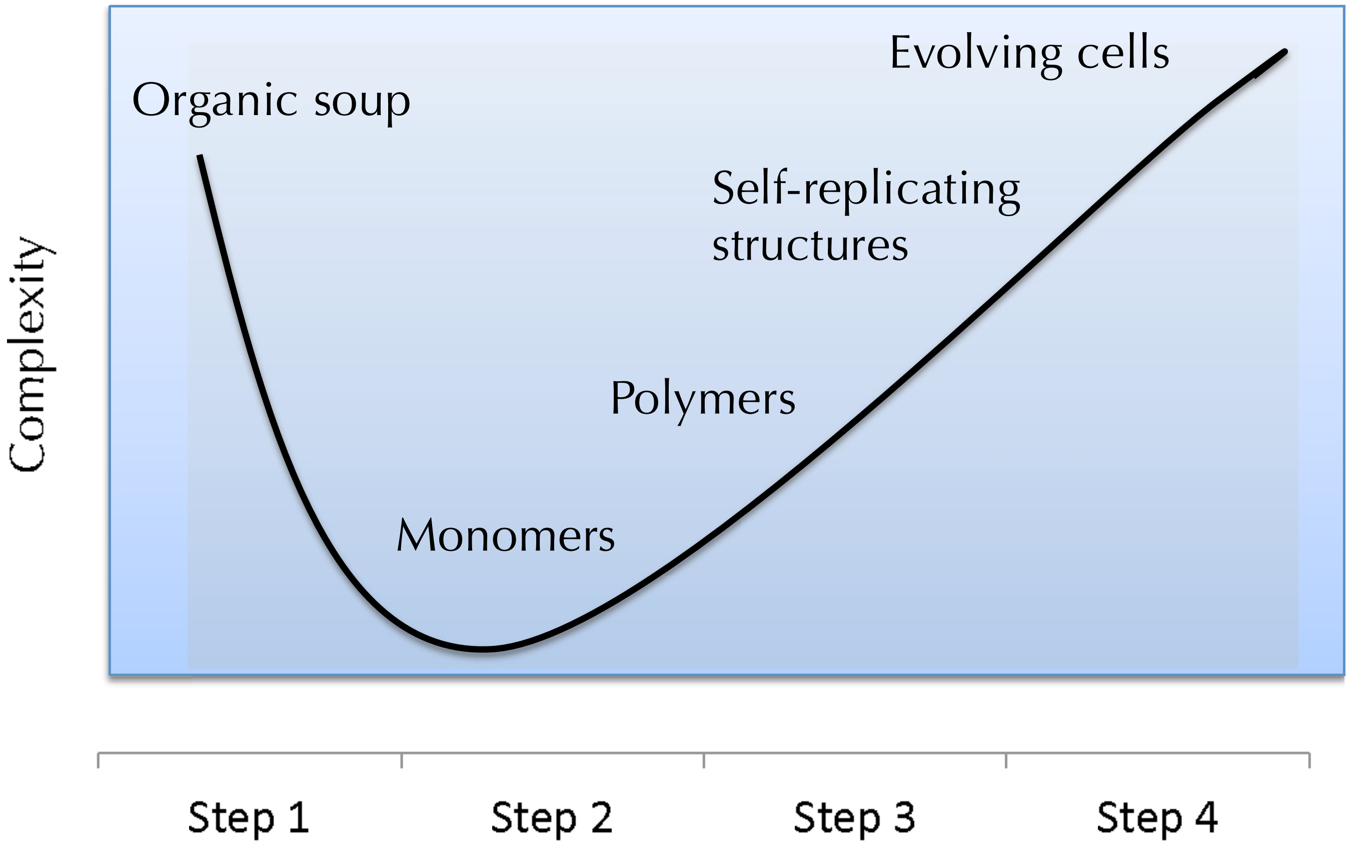
Self-moving systems and the origin of life

- Hypothesis: Life started simple and became more and more complex

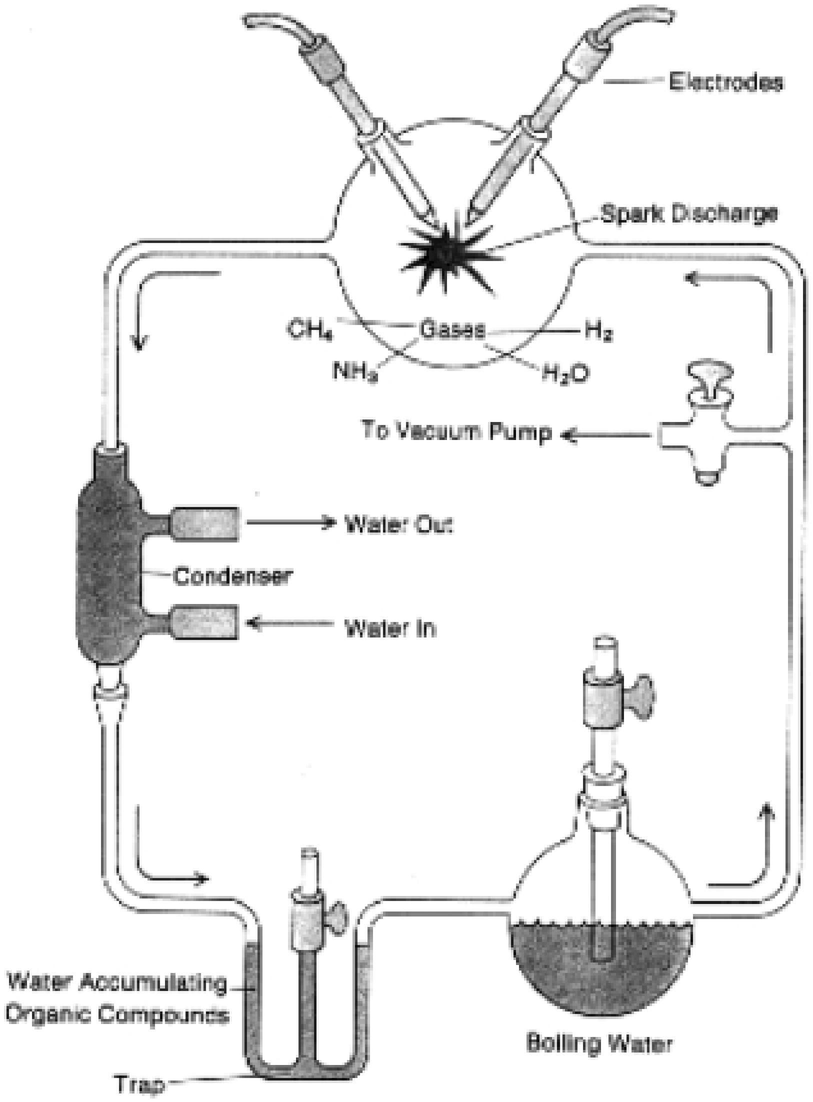


Self-moving systems and the origin of life

- Hypothesis: Maximalism
  - Ikegami T and Hanczyc MM. 2009.. Technoetic Arts Journal,Vol. 7.2, pp153-164.



The Urey-Miller experiment: 1953

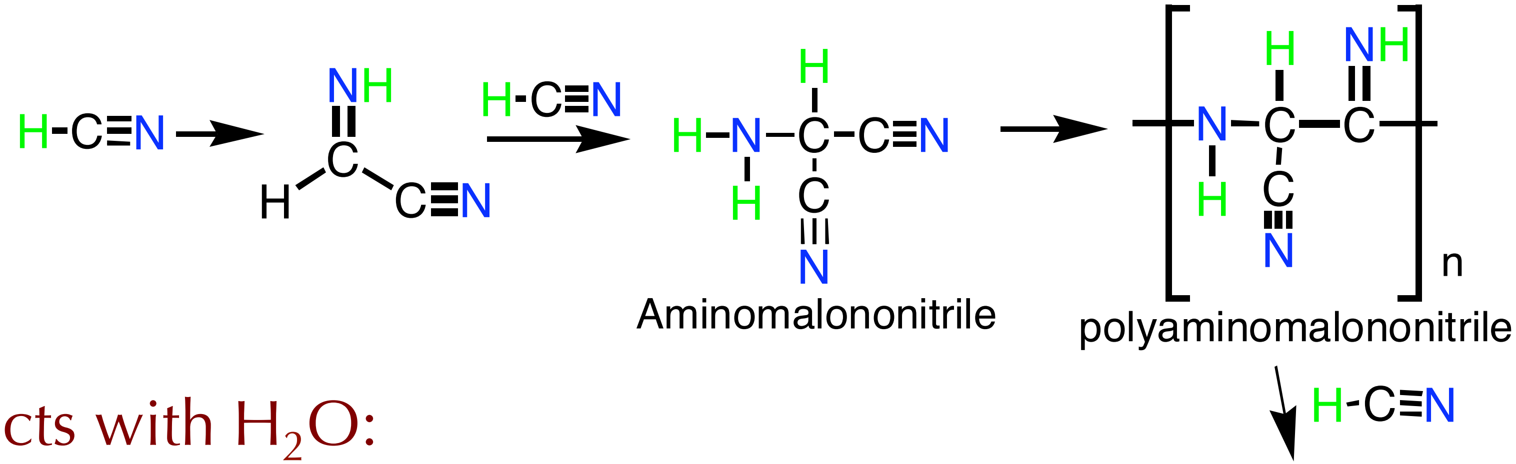


Analysis of molecules in 'ocean': Amino acids, the building blocks of proteins (up to 4%), ***after*** acid hydrolysis.

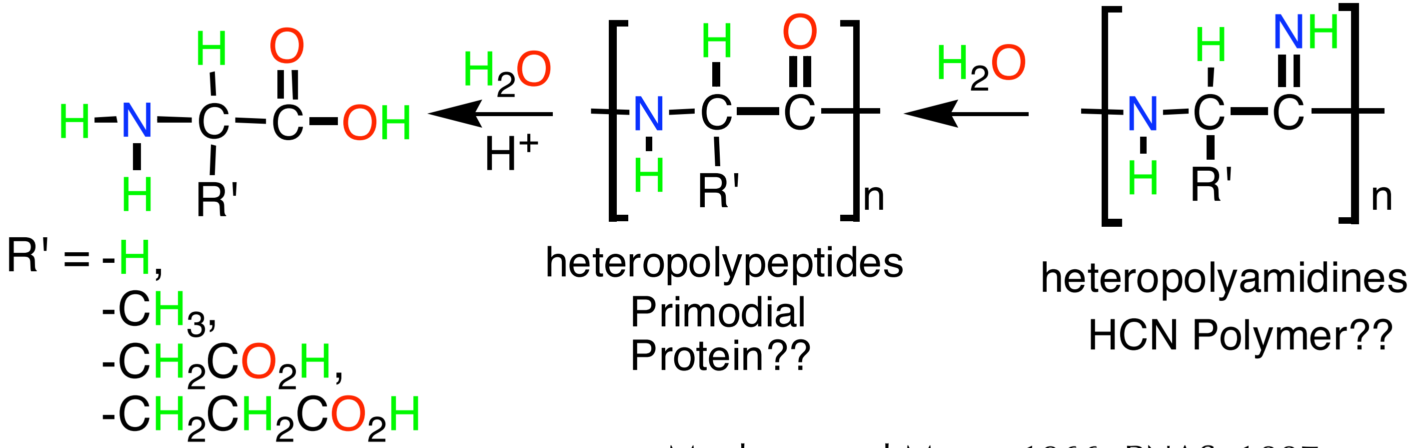
Tar-like substances produced from largely uncontrolled geochemical, atmospheric, and interstellar processes

HCNx

Liquid HCN (bp 25°C) polymerizes spontaneously to a dark brown or black solid at ambient temperatures in the presence of a base such as an amine or ammonia. Matthews and Minard, 2006



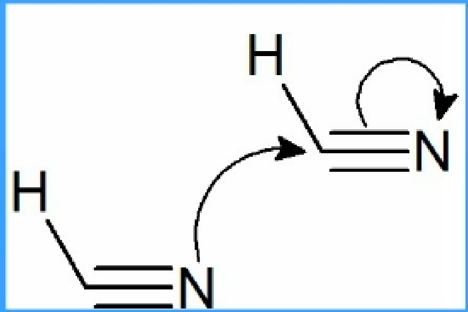
Products with H_2O:

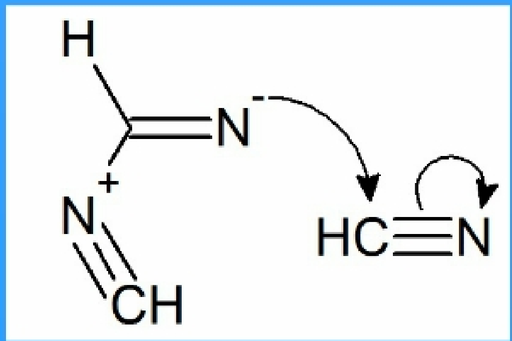


Matthews and Moser, 1966, PNAS, 1087

Dimer Structure: Evans et al. 1991, J. Am. Chem. Soc. 7261

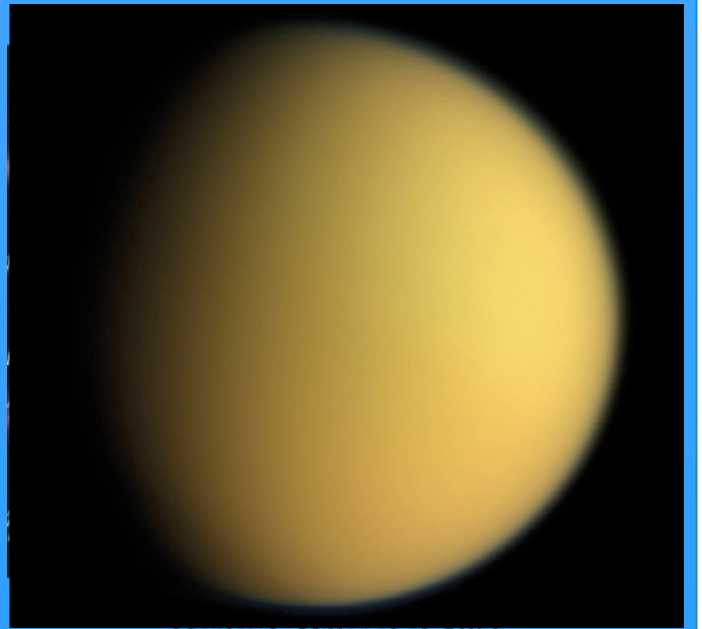
Hydrogen cyanide polymers;





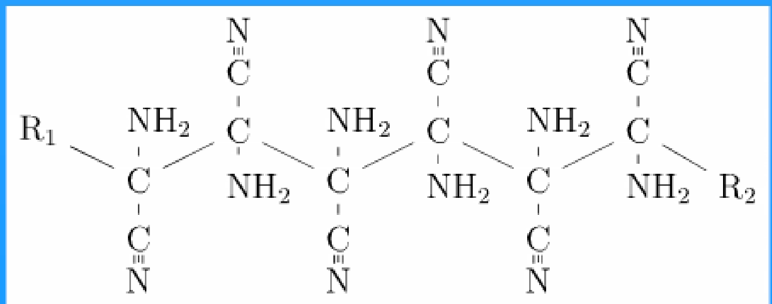
http://en.wikipedia.org/wiki/File:Comet-Hale-Bopp-29-03-1997_hires_adj.jpg

Karen Magee-Sauer et al 1996

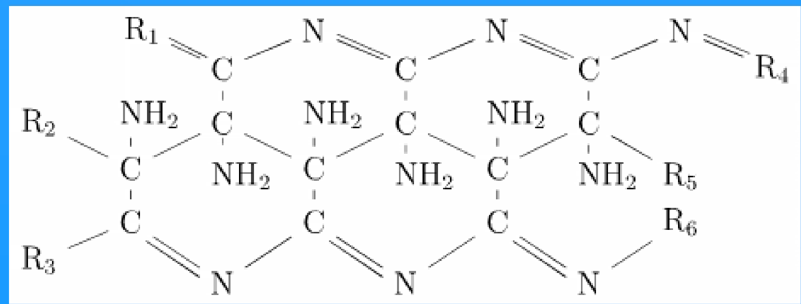


Stanley L. Miller et al. 1955

Titan: largest moon of Saturn

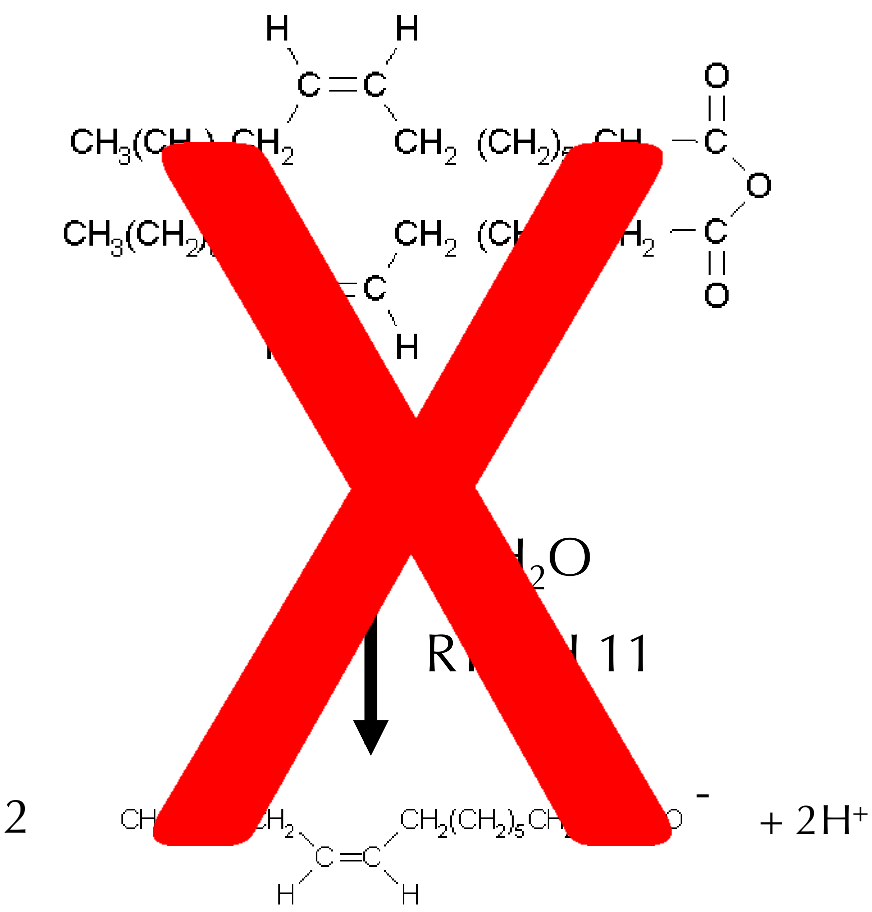


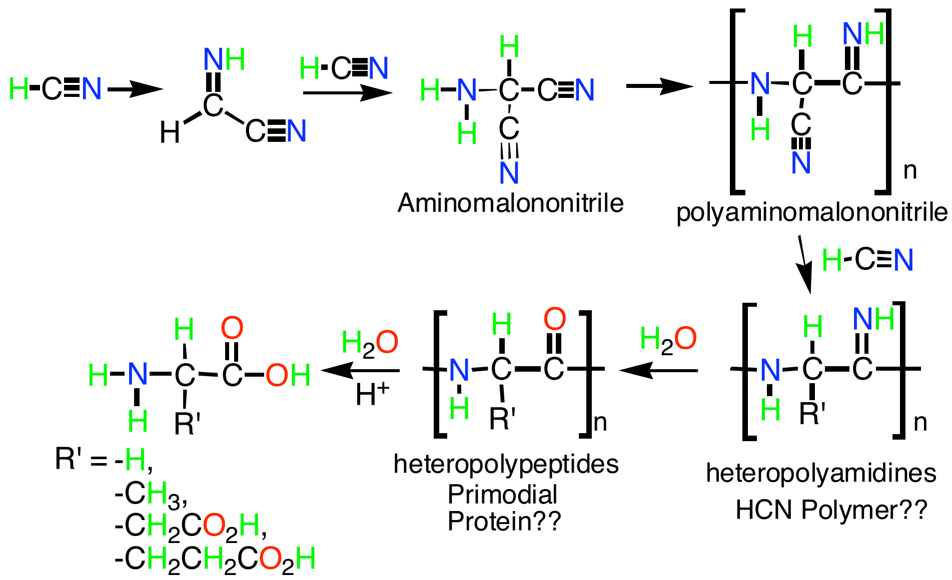
Robert D. Minard et al. 1998



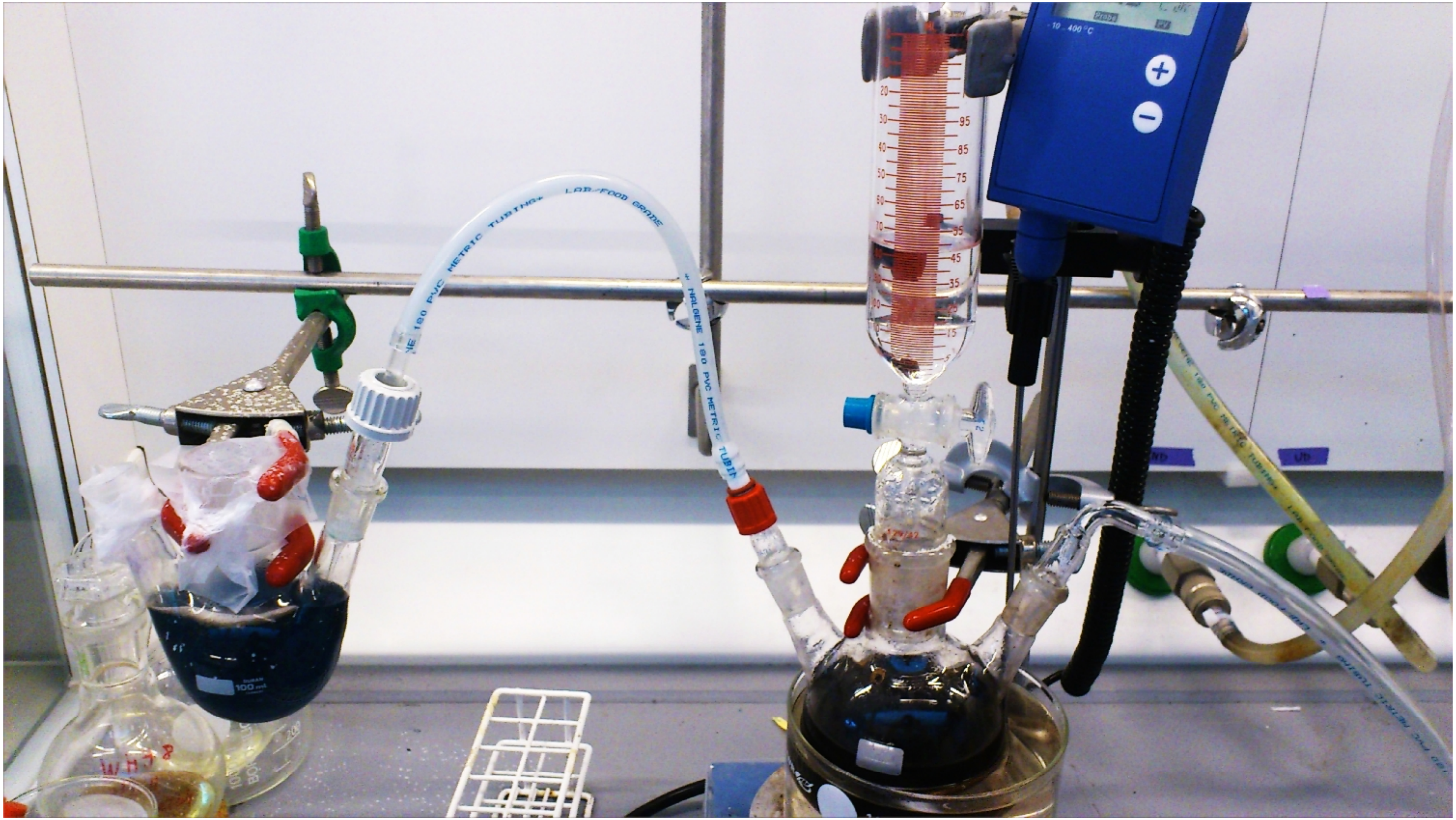
Irena Mamajanov et al. 2009

The Embedded Chemistry





Polymerizing HCN from NaCN in water with HCl addition…

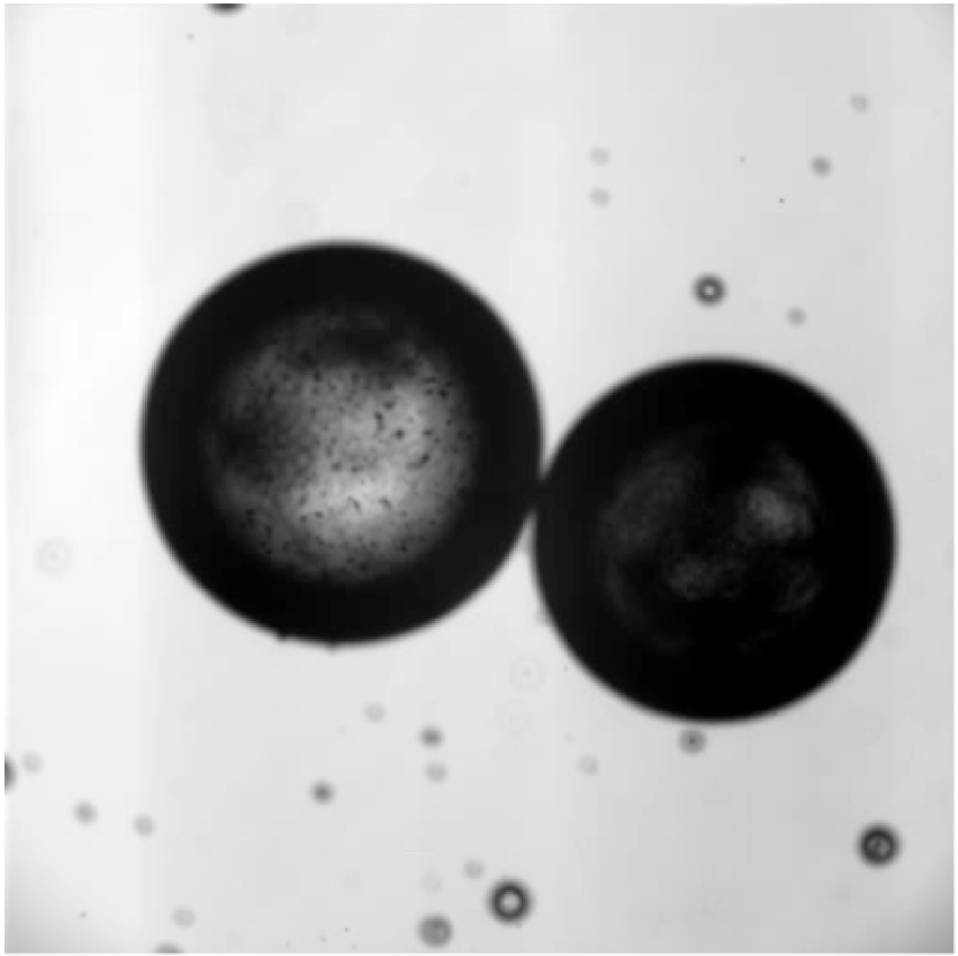


Polymerizing HCN from NaCN in water with HCl addition…

HCN polymer can support movement

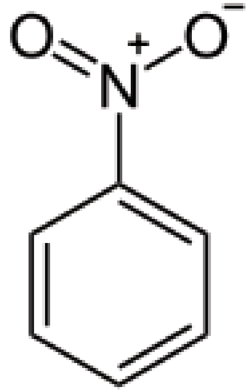
100ul 10mM oleate pH 11

1ul (total) nitrobenzene with 10mg/ml HCN polymer



250 um

OIL:



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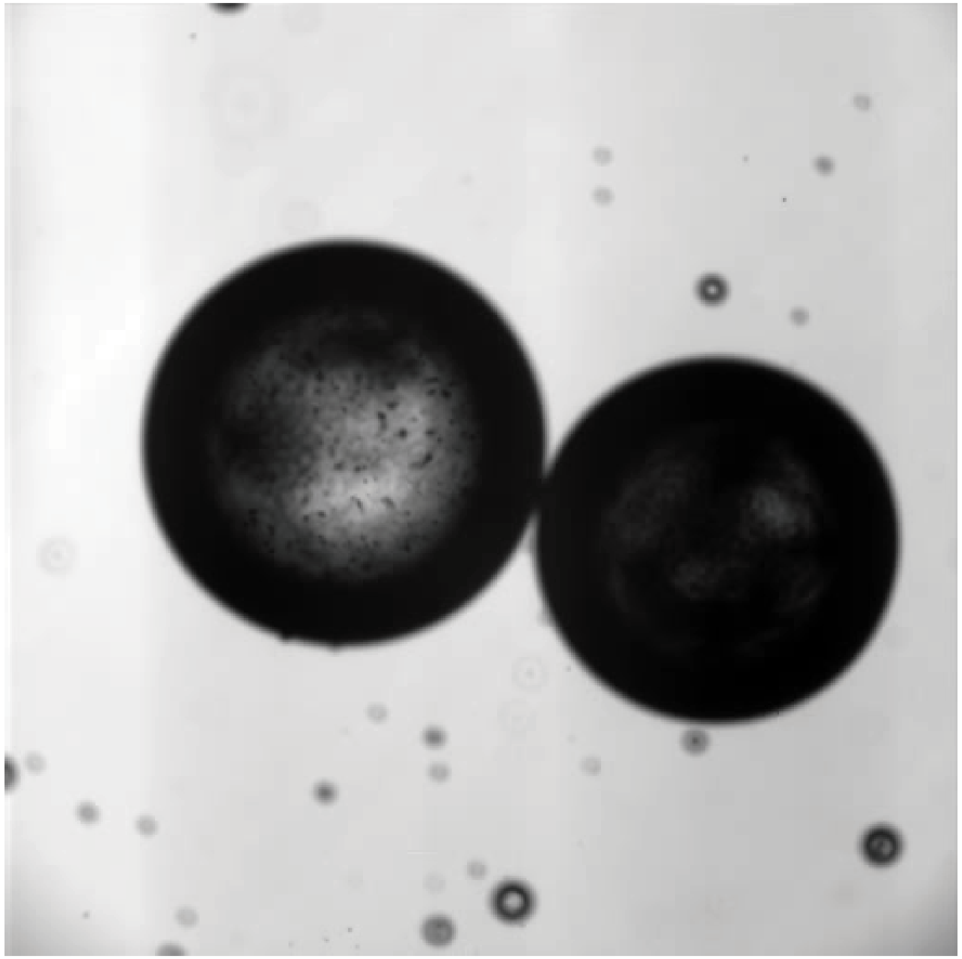
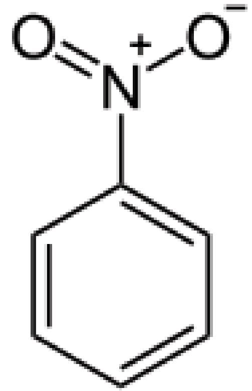


http://youtu.be/JoHtcMuTKRo

250 um

OIL:



HCN polymer can support chemotaxis

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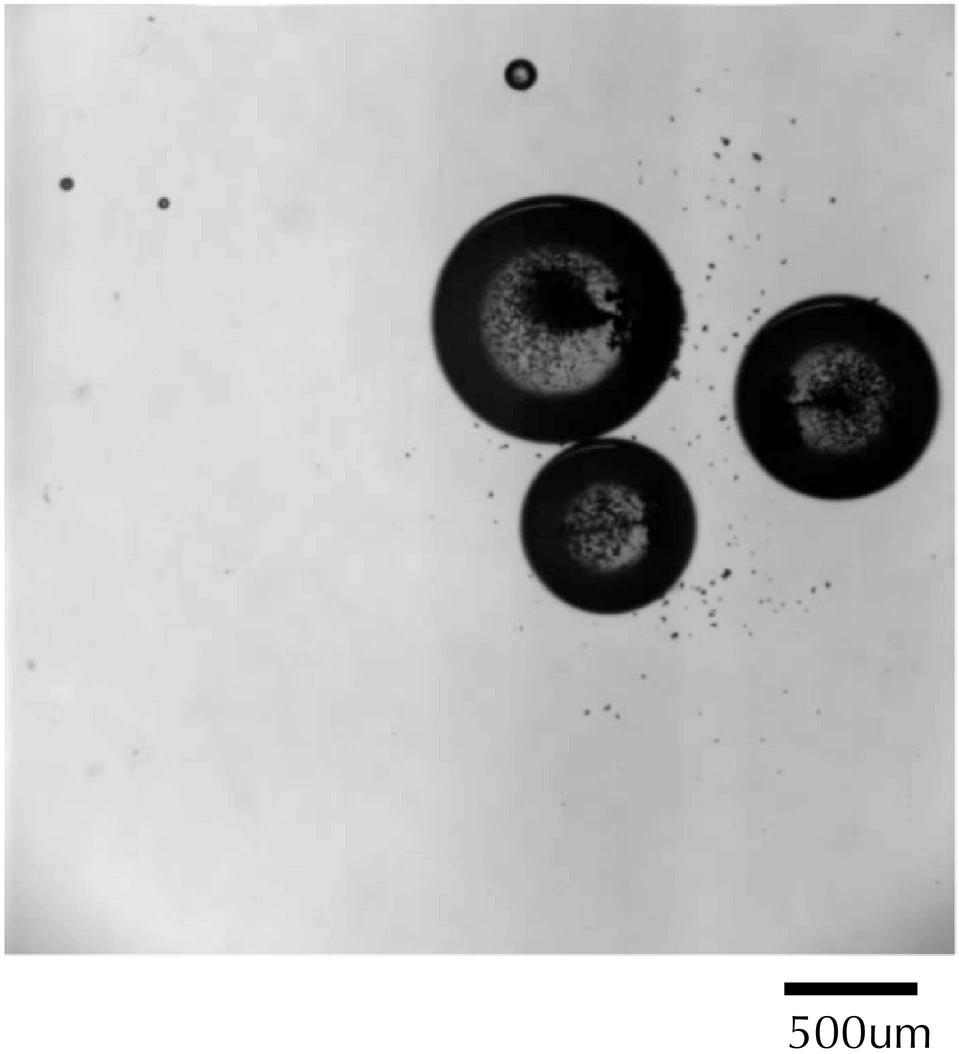
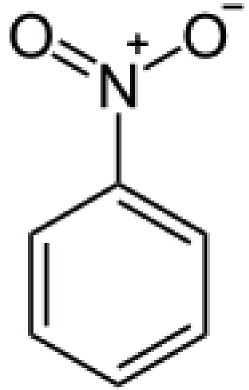
gradient: 1ul 5M NaOH





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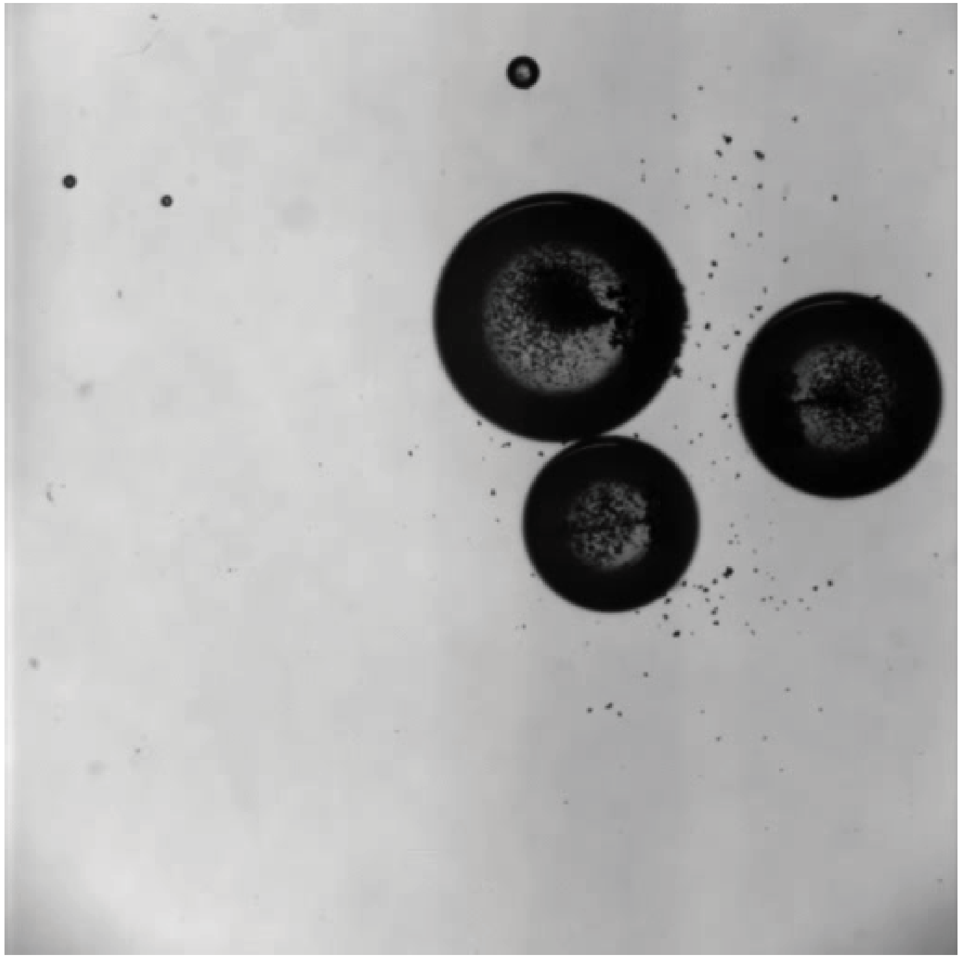

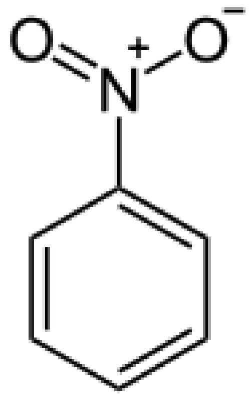

http://youtu.be/Tw9jk9m01XI

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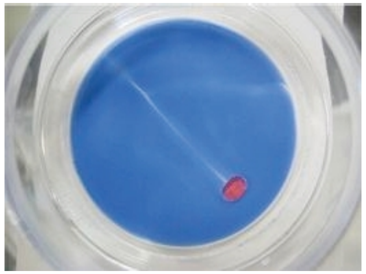
Published online 23 February 2011 | Nature | doi:10.1038/news.2011.118

News

Oil droplets mimic early life

Lack of genetic material no hindrance to life-like behaviour.

Jo Marchant



Dead or alive: could inorganic drops of oil be a precursor to life?

Martin Hanczyc

Oil droplets that creep purposefully through their watery environment, metabolize fuel, sense their surroundings and perhaps even replicate — could these be precursors to life? That's the claim of a chemist with a controversial approach to modelling how Earth's first organisms scraped themselves together.

Theories about how life started range from fortuitous chemistry around hydrothermal vents on the sea floor to the delivery of precursor molecules from outer space. But there is little hope of finding geological evidence for this momentous event: Earth's crust is continuously being recycled, with the oldest known rocks dating to only 3.8 billion years ago. By that point, life was flourishing and relatively complex.

So another way to investigate what happened is to try repeating it — to build basic life forms, called protocells, in the lab. Attempts to do this have generally involved using stripped-down versions of biological cells, and have assumed that certain building blocks, such as RNA, are already present. But Martin Hanczyc at the University of Southern Denmark in Odense is looking for life-like behaviours somewhere much simpler: in drops of oil. He described his work at a Royal Society discussion on the origins of life, held in London on 21 February.

Oily character

Hanczyc's first round of experiments used nitrobenzene oil. To give the droplets a 'metabolism', he put them into a highly alkaline solution (pH 12) and fuelled them with a chemical called oleic anhydride, which converts to oleic acid on contact with water. This

Hanczyc MM. 2011. Metabolism and motility in prebiotic structures. *Phil. Trans. R. Soc. B*, 366, 2885-2893.

Conclusions

- HCNx hydrolysis can support self-movement and chemotaxis
- The fuel is not explicitly defined
- The oil droplet is a simple self-assembled structure powered by prebiotic chemistry and avoids equilibrium

Hydrogen cyanide and the computational origin of life

Conclusions:

The level of chemical complexity that the origin of life had to deal with was enormous.

We can replicate this chemical complexity in the lab with hydrogen cyanide polymerization.

However, what kind of chemical system is it? What are the chemical pathways? This this level of complexity too large to study and understand?