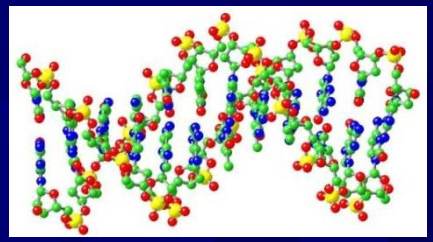
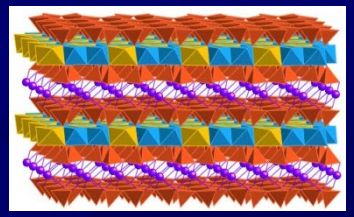
The Origin of Life:
A Battlefield for Dueling Worldviews

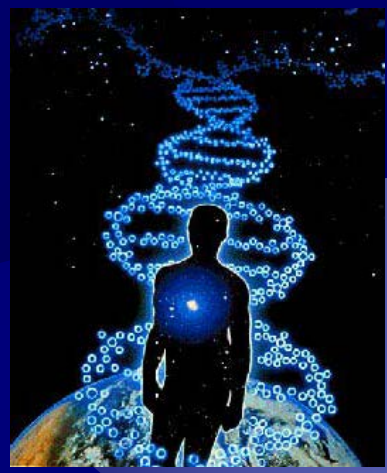
Dr. Scott A. Chambers
Physical & Computational Sciences Directorate
Pacific Northwest National Laboratory
Richland, WA USA

The origin of life – an important and interesting question

- Fascinating scientific questions:
  1. What were the conditions like on early earth?
  2. What synthetic pathways were involved?
  3. Where did the coded information in living systems come from?
- Important implications for worldview:
  1. Does life have a purpose?
  2. Do I as an individual have a purpose?
  3. How is purpose connected to origins?

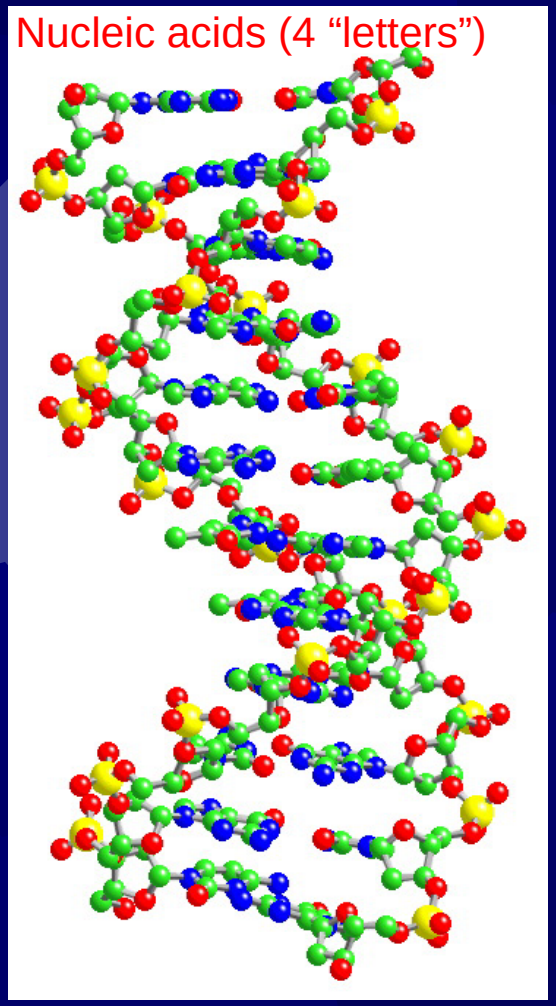


"If human beings (and their beliefs) really are the mindless products of their material existence, then everything that gives meaning to human life – religion, morality, beauty – is revealed to be without objective basis." John J. West, Jr., political scientist, Seattle Pacific University.

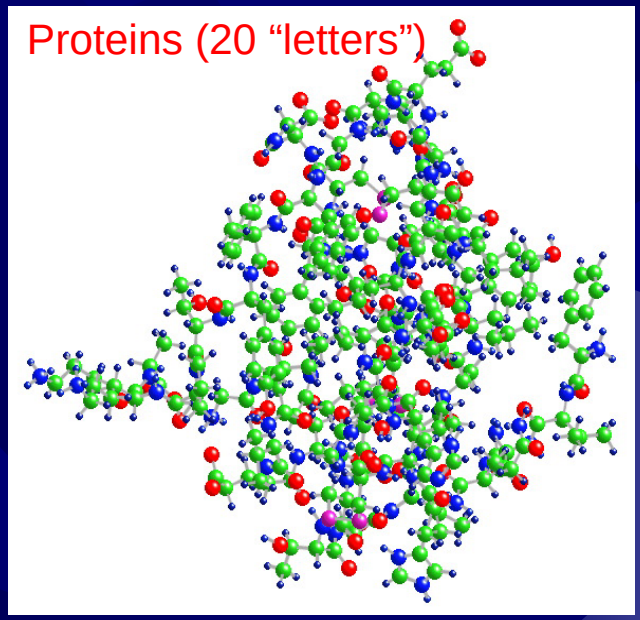
"No life after death; No ultimate foundation for ethics; No ultimate meaning for life; No free will!". William Provine, biologist, Cornell University (deceased) .

Biological polymers – Carrying the coded information required to enable life

Nucleic acids (4 “letters”)

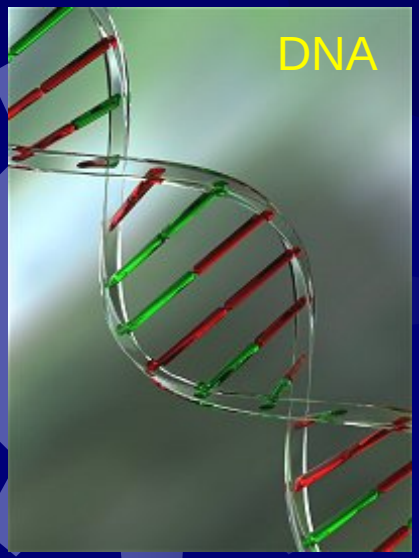


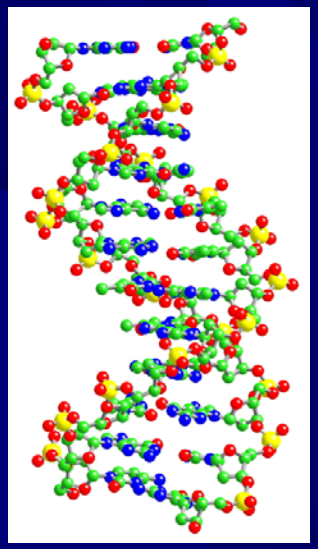
Proteins (20 “letters”)

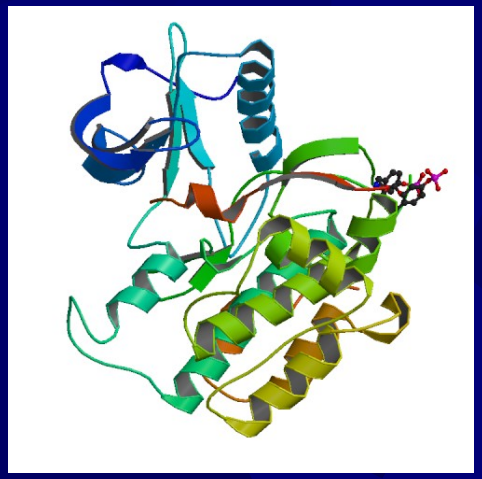


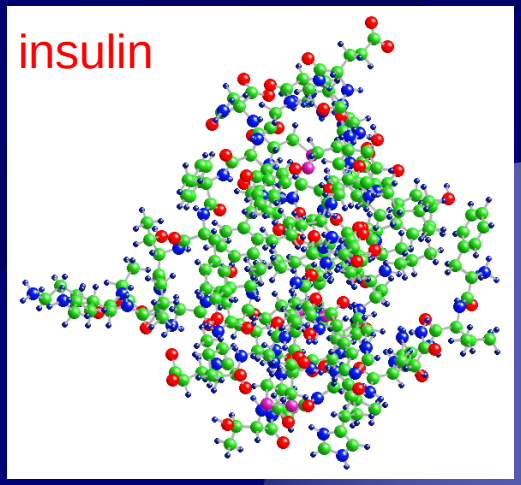
A complex interdependency

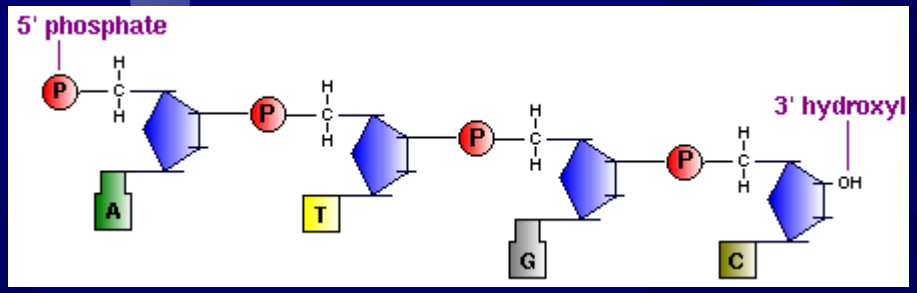
nucleic acids ← catalyzed duplication — proteins



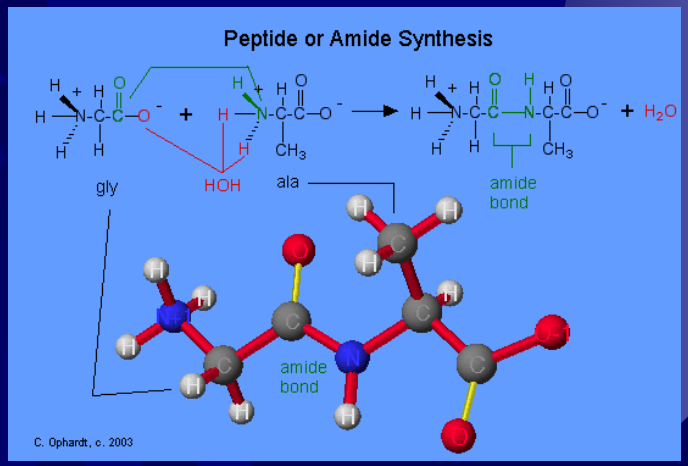






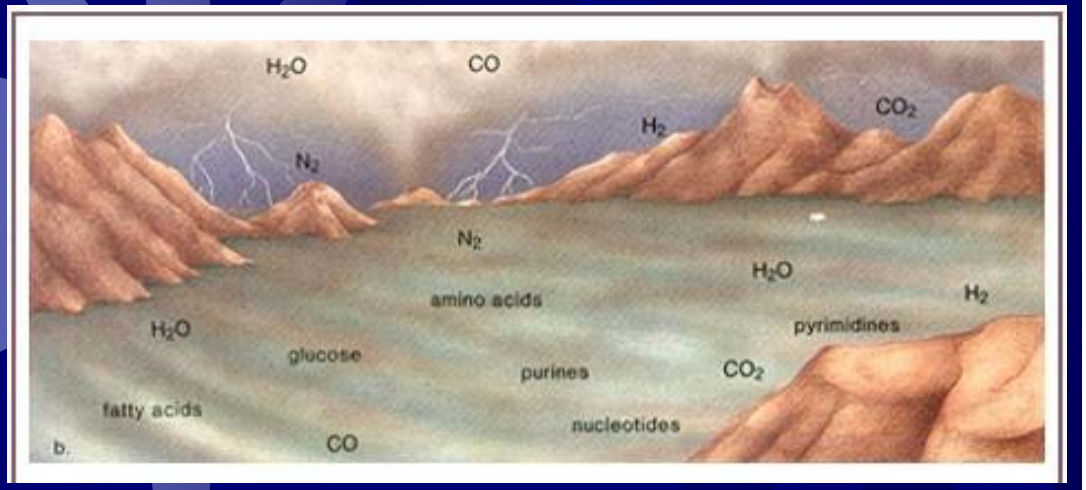


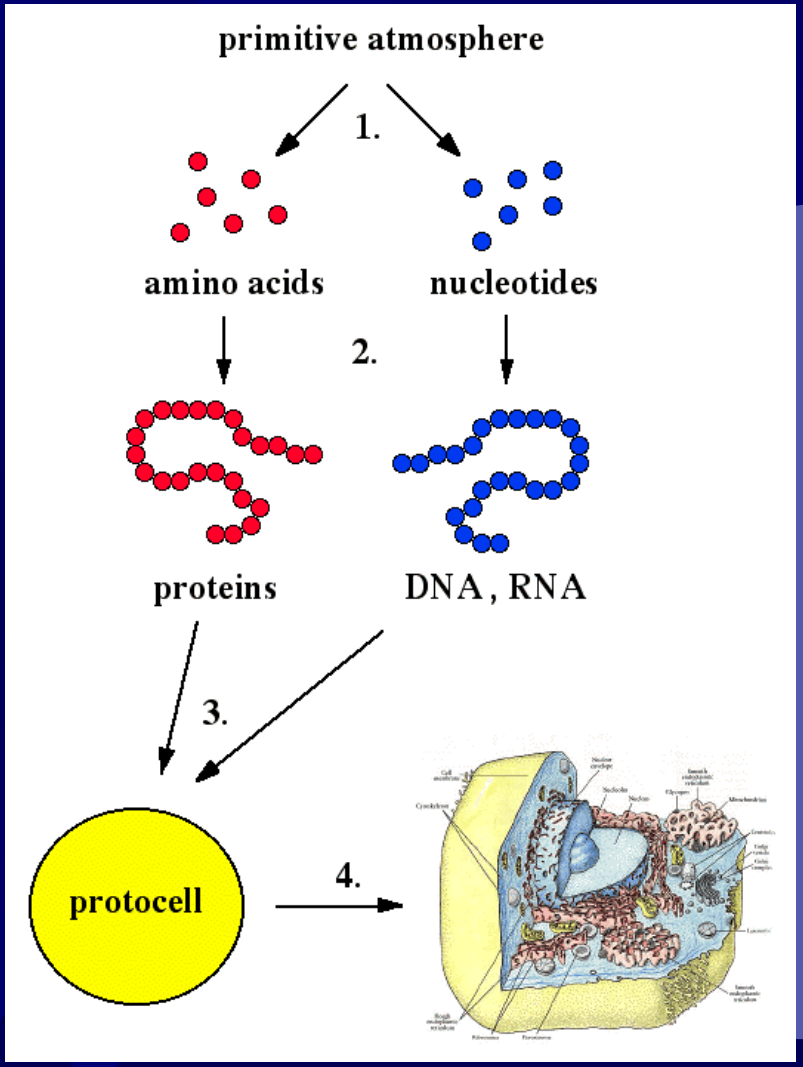
3-5 phosphodiester linkages



linear peptide linkages

The Oparin-Haldane hypothesis

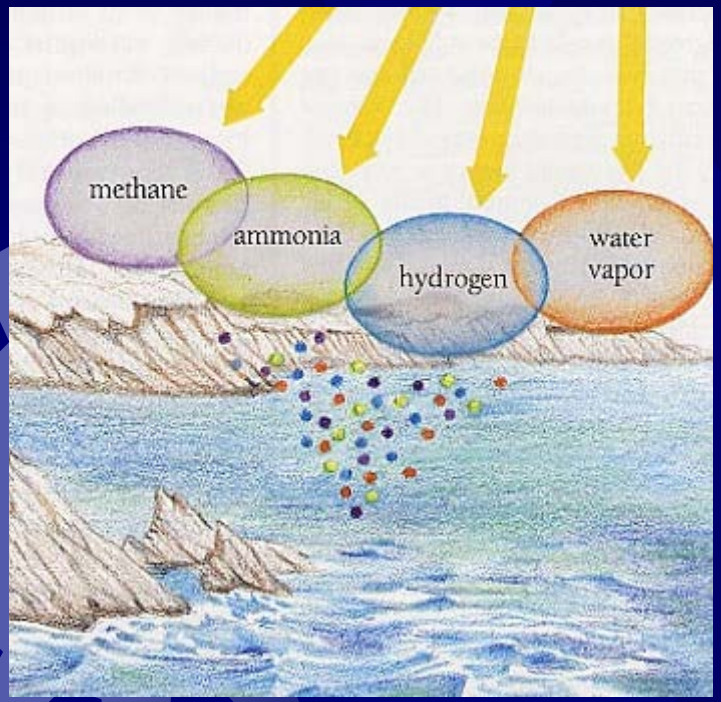




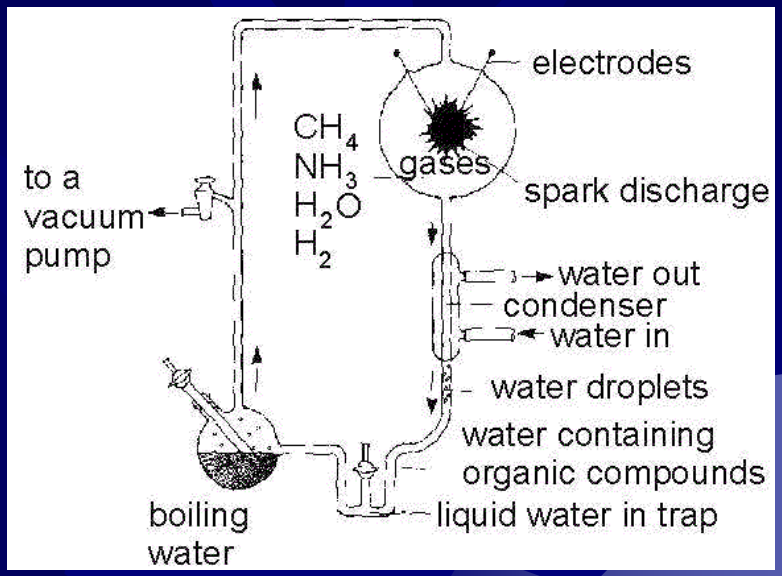
The Oparin-Haldane hypothesis analyzed

- Biomonomer synthesis simulations
- Biopolymer synthesis simulations
- Classical & statistical thermodynamic considerations
- A role for mineral surfaces?
- What’s missing?

Biomonomer formation simulations



The Miller-Urey experiment



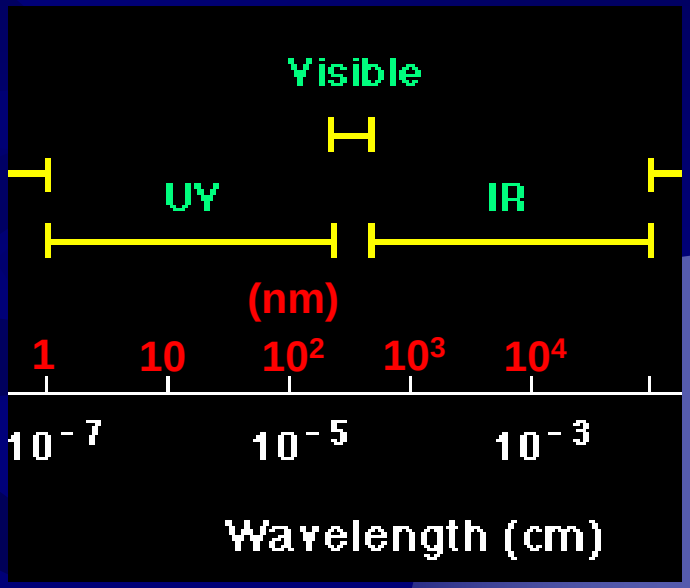
"Approximating conditions on the early earth in a 1952 Experiment, Stanley Miller – now at UCSD – produces amino acids."
National Geographic, March 1998

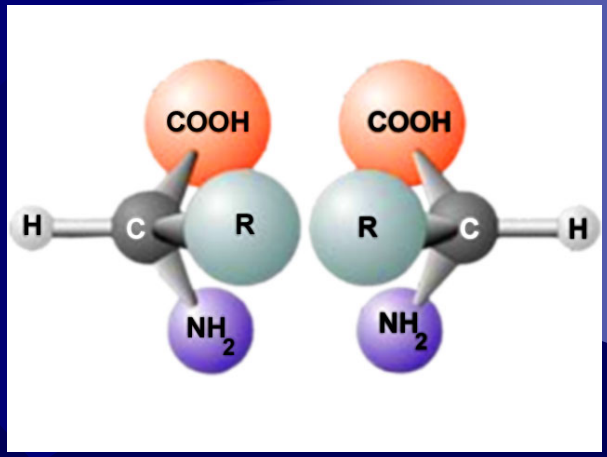
"This research is both a link to the experimental foundations of astrobiology as well as an exciting result leading toward greater understanding of how life might have arisen on Earth." (W. Carl Pilcher, director of the NASA Astrobiology Institute.)

"By recreating the early atmosphere and passing an electric spark through the mixture, Miller and Urey proved that organic matter such as amino acids could have formed spontaneously."
K. Miller and J. Levine, *Biology,* 2000 edition (HS text)

Analysis of the Miller-Urey simulations

- Assumed atmosphere (CH_4, NH_3, H_2O, H_2 - no O_2) unrealistic
  O_2 was present early on (oldest rocks on earth are fully oxidized; Australian zircons, $U_xZr_{1-x}SiO_4$, 4.35 Byr old)
- H_2 present in trace amounts only (easily lost to space)
  No H_2 → no NH_3 or CH_4
  "The strongest evidence (for a reducing atmosphere) *is provided by conditions for the origin of life. A reducing atmosphere is required."* J.C.G. Walker, *Evolution of the Atmosphere* (1997).
  "…the early atmosphere looked nothing like the Miller-Urey simulation." Jon Cohen, *Science* (1995).
- Only light of wavelength less than 200 nm (~0.01% of solar spectrum) was used. No light from 200 and 400 nm (~11% of solar spectrum) was used.
  Light in this range photodissociates amino acids.
- Traps were used to isolate and protect products.
  No traps present in the prebiotic atmosphere.
- Only racemic mixtures of amino acids were formed (*L* and *D*, or left- and right-handed).
  All "living" proteins use only left-handed amino acids.
- *Simulations worked because of the infusion of design*





More recent work

John Sutherland group (Cambridge)

- Three important classes of biomonomers (nucleic acids, amino acids and lipids) can be made from HCN, H_2S and UV light (Patel *et al.,* Nat. Chem. **7**, 301 (2015)).
- HCN found in comets. H_2S believe to be present on early earth.
- Different conditions required to make these three kinds of biomonomers – not likely made at same time or same place – but…" *Rainwater would then wash these compounds into a common pool*," (Dave Deamer, origin-of-life researcher, University of California, Santa Cruz).

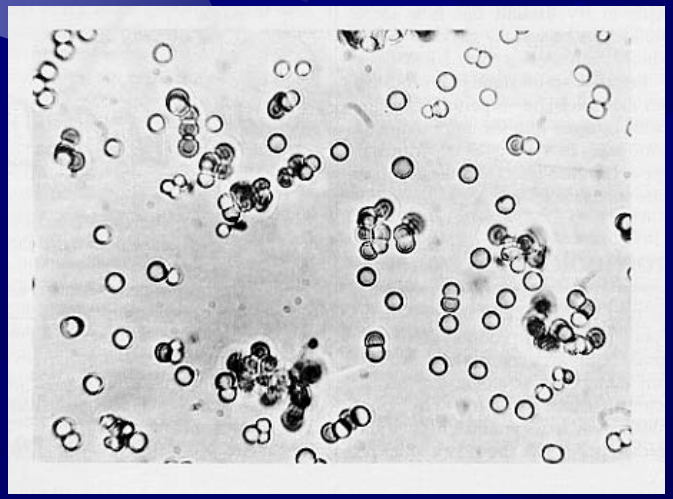
Issues of relevance:

- Highly controlled conditions.
- Photochemically specific UV wavelengths used.

Biopolymer formation simulations

Sidney W. Fox simulations

dry amino acids —heat, N_2→ polypeptides (proteinoids) —boiling water→ proteinoid microspheres



- Pure, dry amino acids used as starting materials. Other organics (e.g. sugars) would incorporate and form nonbiological “junk”.

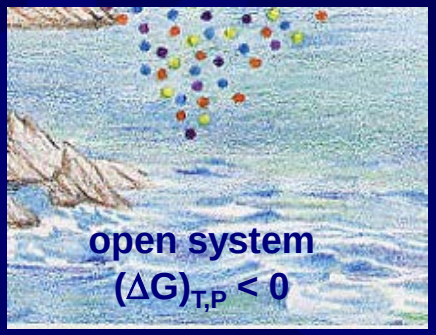
  An “organic soup” in the prebiotic world would contain many kinds of organic molecules.
- Only left-handed amino acids used.

  Equal mixture of left- and right-handed amino acids would have been present in the natural environment.
- No water allowed until after polypeptide formation.

  Water would reverse the reaction according to the law of mass action ($A + B = AB + H_2O$).
- No oxygen allowed.

  Oxygen would destroy the product.
- No linear polypeptides formed.
- Minimal catalytic activity observed for protenoids..
- *Conditions engineered to get results*

Thermodynamics of biopolymer formation



$A + B \rightleftharpoons AB + H_2O$ (dipeptide formation)

$AB + C \rightleftharpoons ABC + H_2O$ (tripeptide formation)

$ABC + D \rightleftharpoons ABCD + H_2O \ldots\ldots \rightleftharpoons$ protein

For each step, need to calculate the free energy change (ΔG)

ΔG^o = free energy difference between products and reactants

$$= \Sigma G_f^o{}_{prod} - \Sigma G_f^o{}_{react}$$

$$= \Delta H^o - T\Delta S^o{}_{th}$$

ΔH^o = enthalpy change

$\Delta S^o{}_{th}$ = thermal entropy change

T = temperature

Equilibrium constant (K)
= ratio of product concentrations to reactant concentrations
For A+B+C+D → ABCD, $K = [ABCD]/[A][B][C][D] = e^{-\Delta G/RT}$

If $\Delta G^o \leq 0$, $K \geq 1$ → more products than reactants (spontaneous)
If $\Delta G^o > 0$, $K < 1$ → more reactants than products (not spontaneous)

Spontaneous polypeptide formation?

$A + B \rightleftharpoons AB + H_2O$ (dipeptide formation)

$AB + C \rightleftharpoons ABC + H_2O$ (tripeptide formation)

$ABC + D \rightleftharpoons ABCD + H_2O$ (tetrapeptide formation)

ΔG^o = ~3 Kcal/mol per linkage at 25°C

K = ~0.01 (~1% yield per linkage)

For three linkages (formation of ABCD)

ΔG^o = ~9 Kcal/mol

K = ~3 x 10^{-7}

75 molecules ABCD per billion molecules (each) of A, B, C, D

Statistical thermodynamic considerations

Must consider the sequence of biomonomers → configurational entropy (ΔS_c)

$2A + 2B \rightarrow A_2B_2$

1.	*A-A*-B-B**	*A-A-B-B*
2.	*A-A*-B*-B*	
3.	*A*-A-B-B**	
4.	*A*-A-B*-B*	
5.	*B-B*-A-A**	*B-B-A-A*
6.	*B-B*-A*-A*	
7.	*B*-B-A-A**	
8.	*B*-B-A*-A*	
9.	*A*-B*-A-B*	*A-B-A-B*
10.	*A*-B-A-B**	
11.	*A-B*-A*-B*	
12.	*A-B-A*-B**	
13.	*B*-A*-B-A*	*B-A-B-A*
14.	*B*-A-B-A**	
15.	*B-A*-B*-A*	
16.	*B-A-B*-A**	
17.	*A*-B*-B-A*	*A-B-B-A*
18.	*A*-B-B*-A*	
19.	*A-B*-B-A**	
20.	*A-B-B*-A**	
21.	*B*-A*-A-B*	*B-A-A-B*
22.	*B*-A-A*-B*	
23.	*B-A*-A-B**	
24.	*B-A-A*-B**	

Statistical thermodynamic considerations

Number of ways of linking 2 A with 2 B assuming A & B are *distinguishable* = 4x3x2x1 = 4! = 24

Number of ways assuming A & B are *indistinguishable* = (4x3x2x1)/(2)(2) = 6

$\Omega_{rnd} = n_{tot}!/(n_A!n_B!)$

$\Delta S_c = S_{seq} - S_{rnd} = R[\ln\Omega_{seq} - \ln\Omega_{rnd}] = 1.98[\ln(1) - \ln(6)] = -3.6$ cal/mol-deg

$T\Delta S_c = -1$ Kcal/mol at 25°C

$\Delta G^o = \Delta H^o - T\Delta S^o_{th} - T\Delta S_c = 9 + 1 = 10$ Kcal/mol

$K = 5 \times 10^{-8}$

25 molecules A_2B_2 per billion molecules (each) of A & B

For a “real” but small polypeptide (101 amino acids – 100 linkages from 5 each of the 20 amino acids found in biological proteins)

$\Delta G^o = \Delta H^o - T\Delta S^o_{th} - T\Delta S_c$

$\Delta H^o - T\Delta S^o_{th} = \sim 300$ Kcal/mol at 25°C

$T\Delta S_c = T(S_{seq} - S_{rnd})$

$= kN_A T[\ln\Omega_{seq} - \ln\Omega_{rnd}]$

$= kN_A T\{\ln(1) - \ln[(100!/(5!)^{20}]\}$

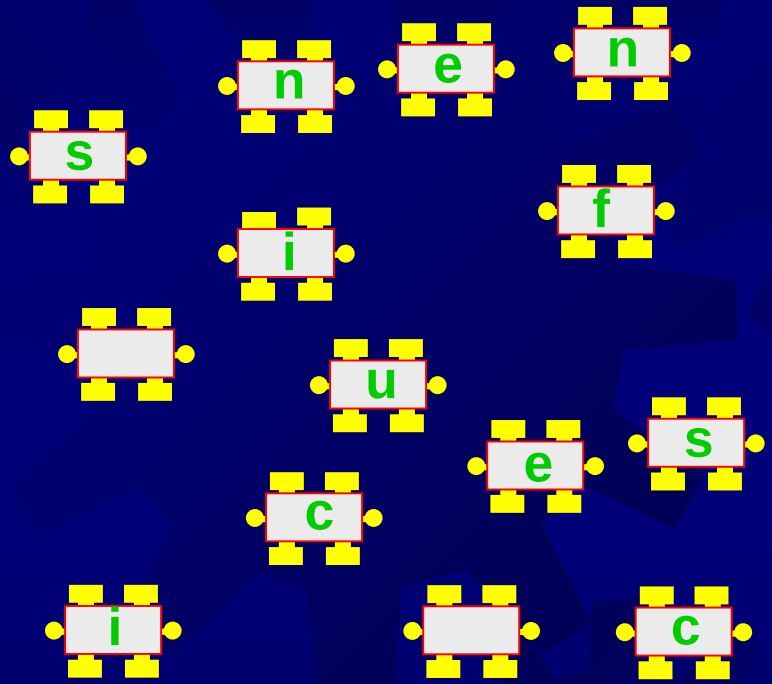
= -157 Kcal/mol at 25°C (assuming a molecular weight of ~10,000)

$\Delta G^o = 300 + 157 = 457$ Kcal/mol at 25°C

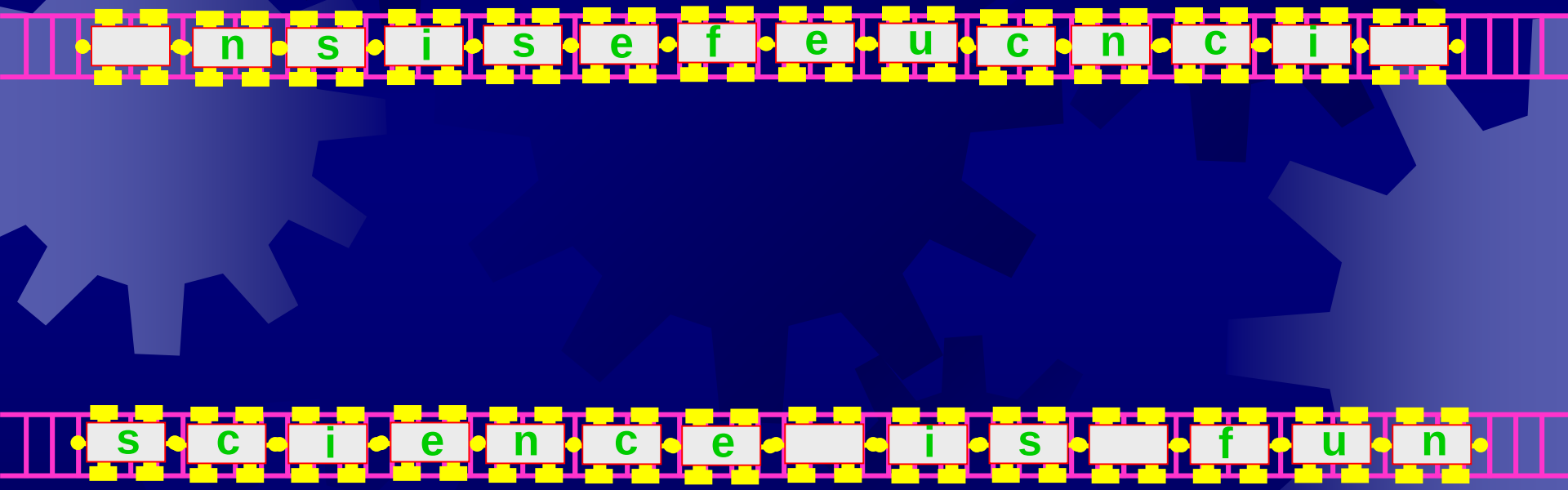
$K = e^{-\Delta G/RT} = \sim 10^{-338} = 0$ (*no polypeptide yield → zero ppb)*

(C.B. Thaxton, W.L. Bradley & R.L. Olsen, *The Mystery of Life’s Origin – Reassessing Current Theories*, Lewis & Stanley, 1984.)

Analogy – a model train



Analogy – a model train



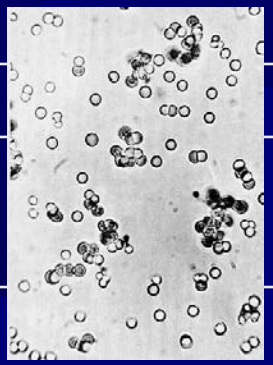
Did crystalline minerals play a role?

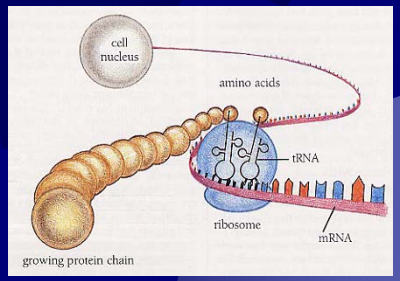
early earth atmosphere	hot dilute organic soup	widescale polymerization	protocells	living cells

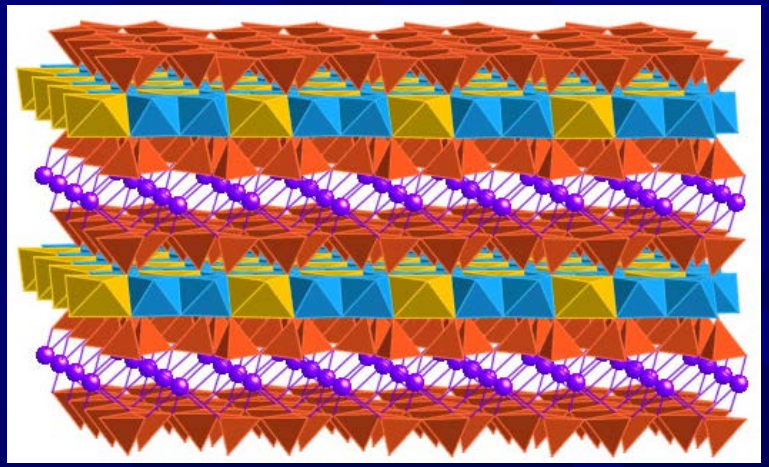
H_2O
H_2
CH4
CO
CO_2
NH_3
N_2

fatty acids → lipids → membranes
amino acids → peptides → proteins

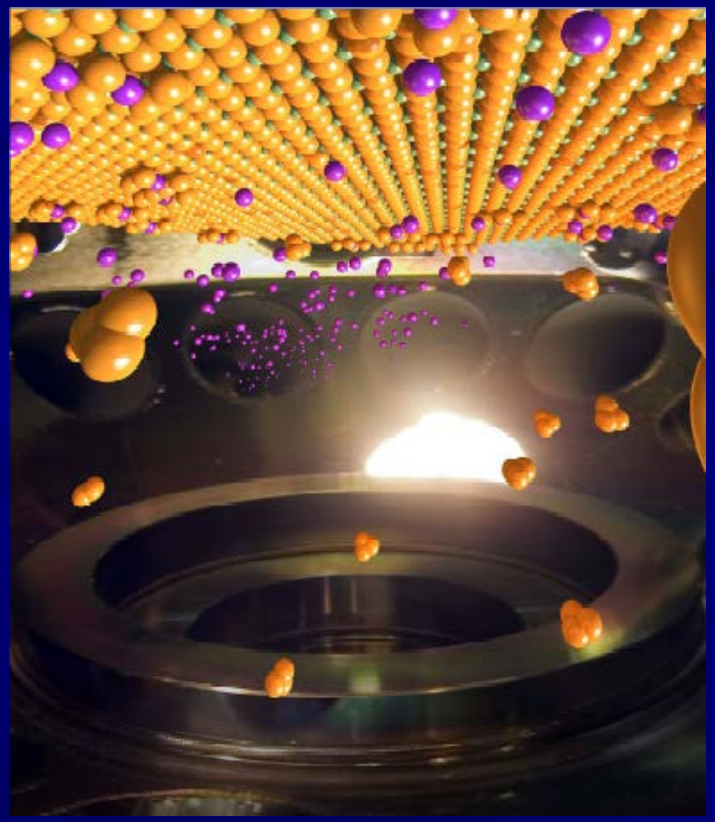
purines
pyrimidines → poly-nucleotides → DNA/ RNA

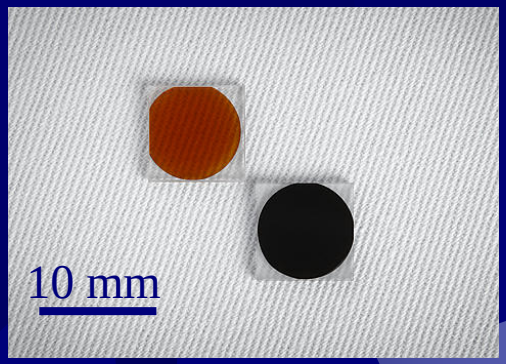


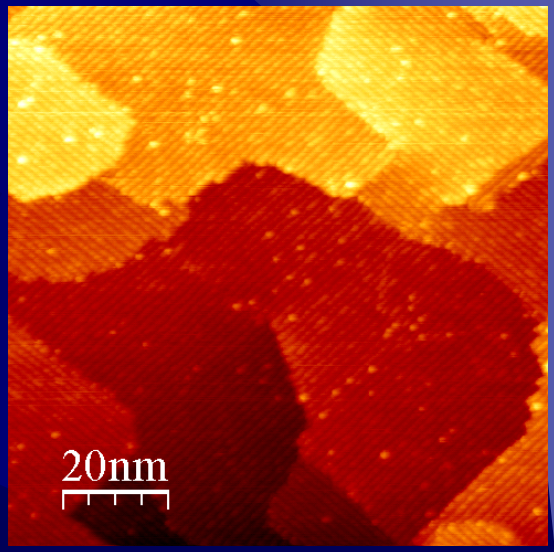




Chemistry of small organics on model mineral surfaces prepared by molecular beam epitaxy*

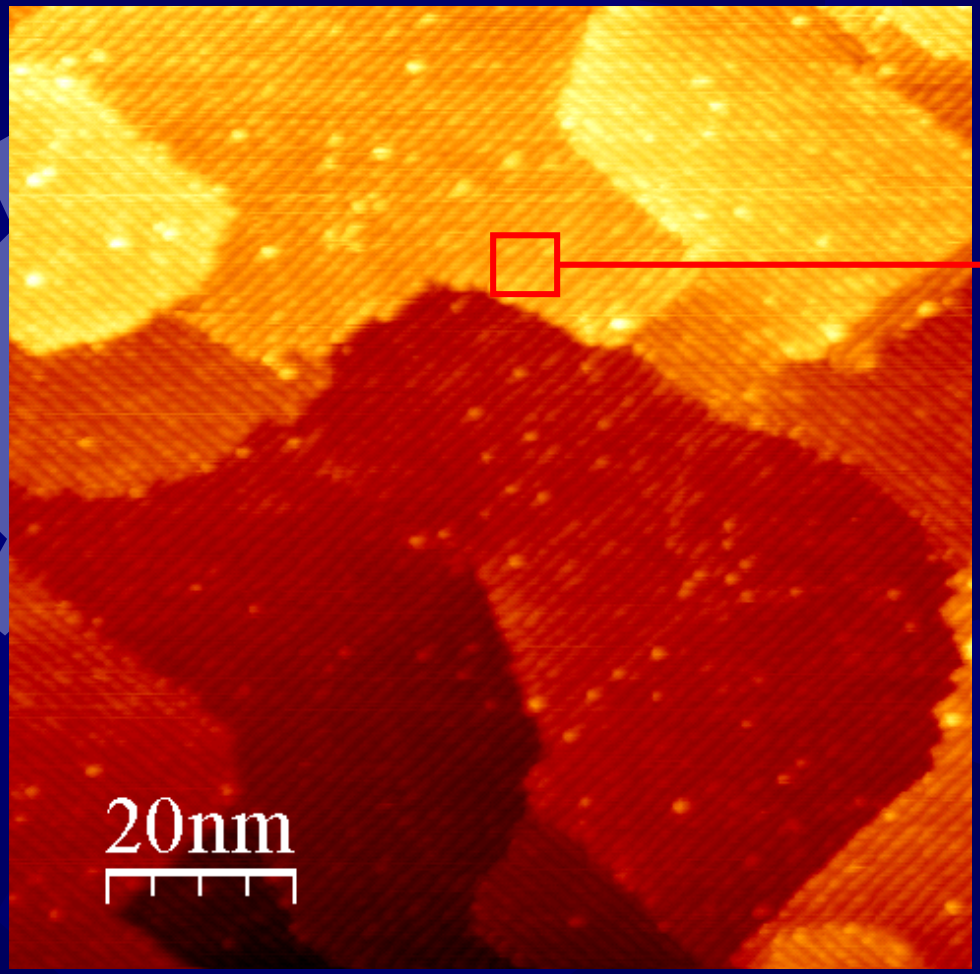


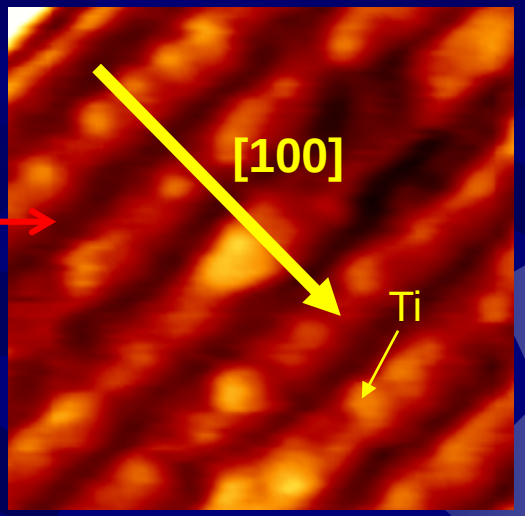


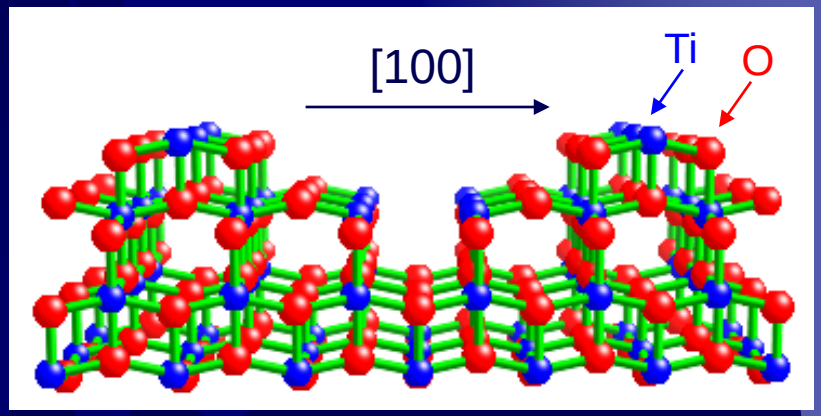


*S.A. Chambers, *Advanced Materials* 2**2,** 219 (2010)

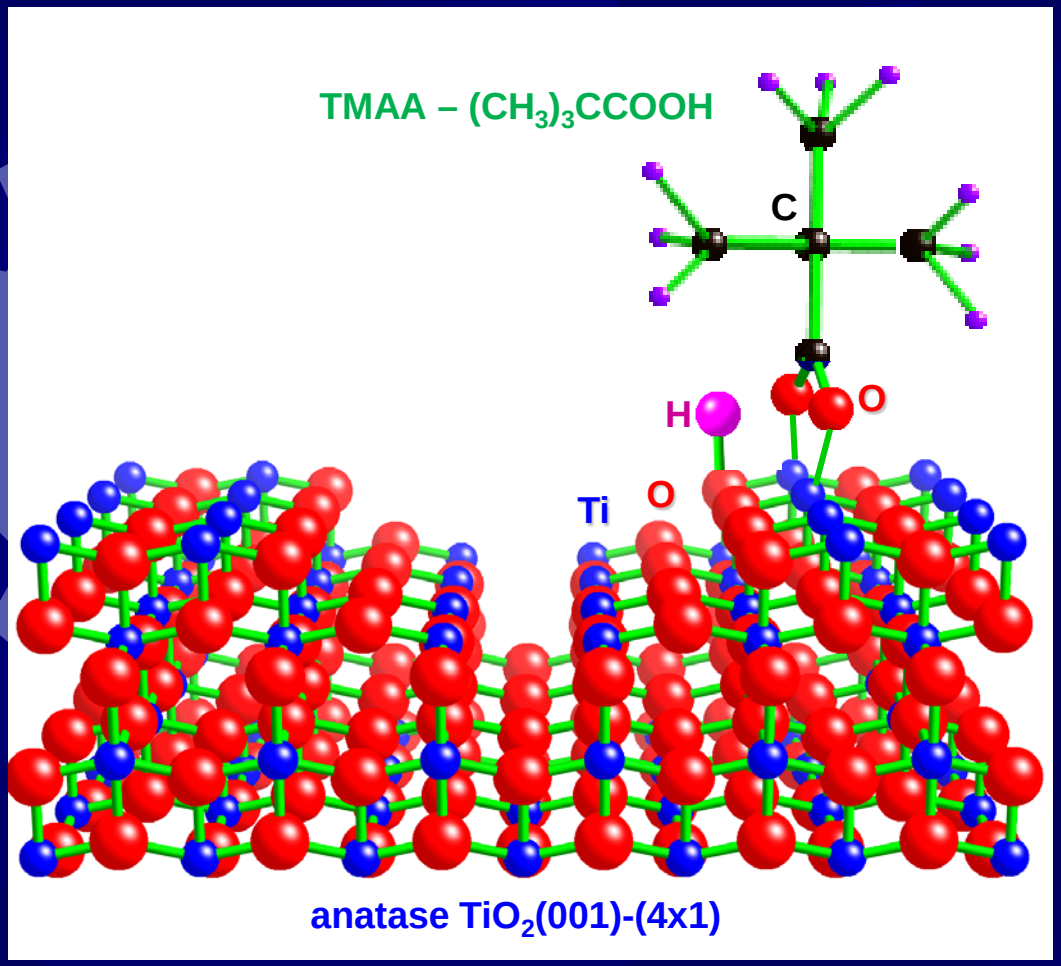
Model surfaces of anatase $TiO_2(001)$



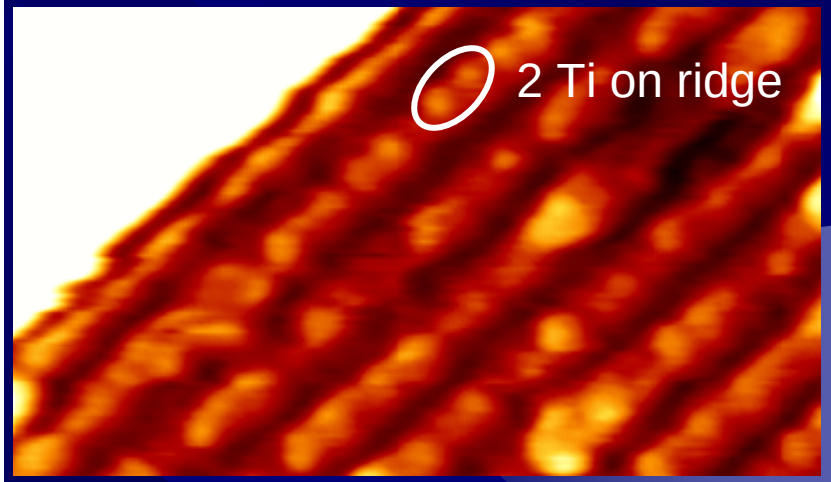




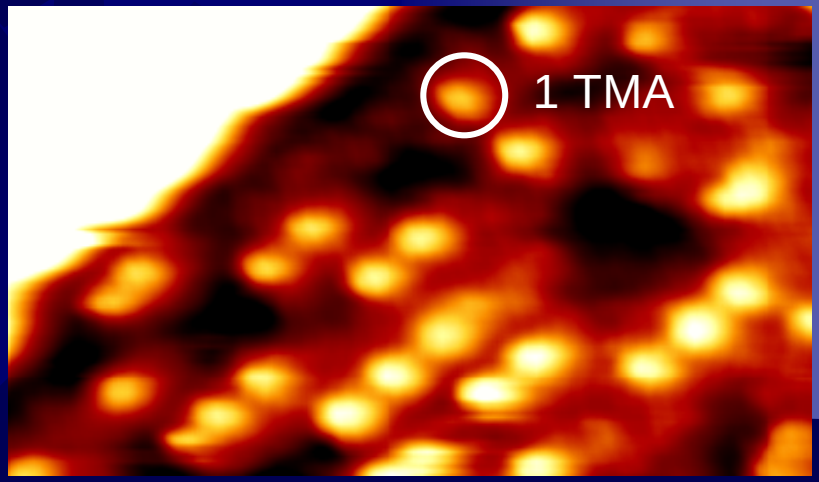
Trimethyl acetic acid (TMAA) on TiO_2(001)



clean TiO_2(001)-(4x1)

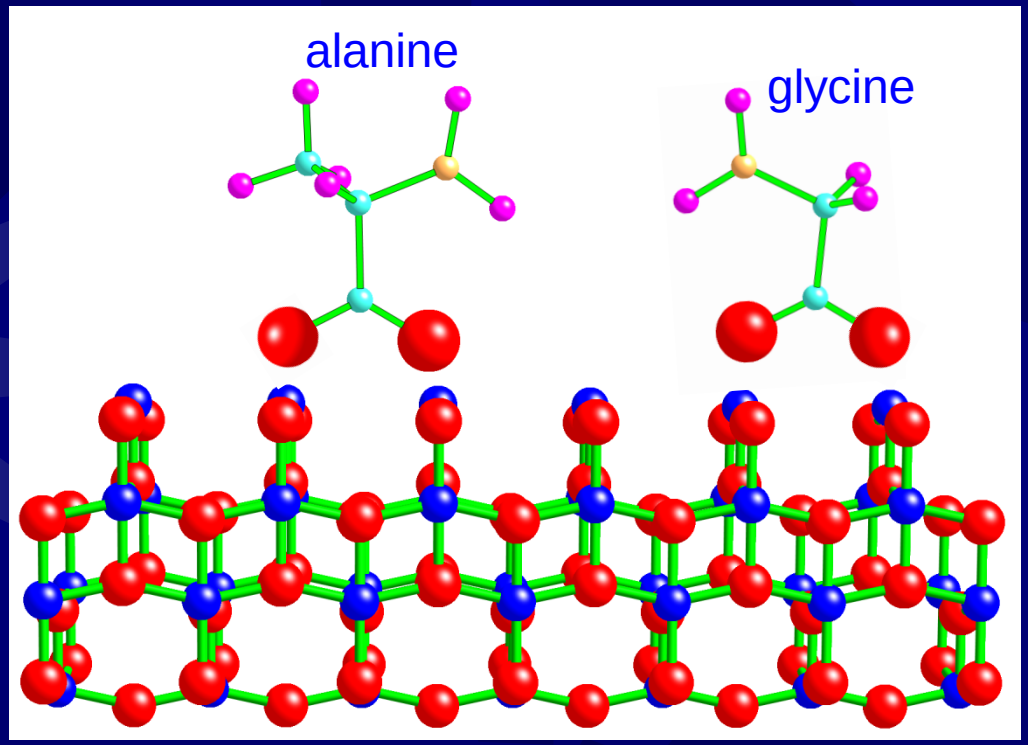


TMA on TiO_2(001)



Ohsawa *et al*., J. Phys. Chem. C **112**, 20050 (2008)

Amino acids on mineral surfaces



- Sorption is via carboxyl groups to surface cations
- Crystallographic order on surface insures uniform spacing
- *No way to generate specific sequences of amino acids*
- *The mineral surface does not carry the required information*

Order vs. complexity

- If a material is ordered – minimal instruction set required to specify the structure

  Characteristic of crystals (e.g. NaCl)

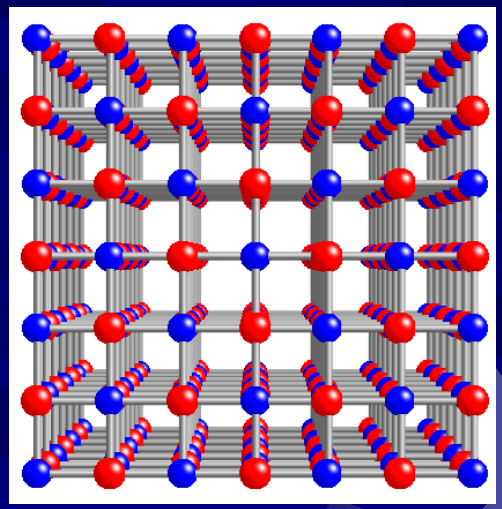
  Information carrying capacity very small

- If a material is complex – large instruction set required to specify the structure

  Characteristic of biopolymers

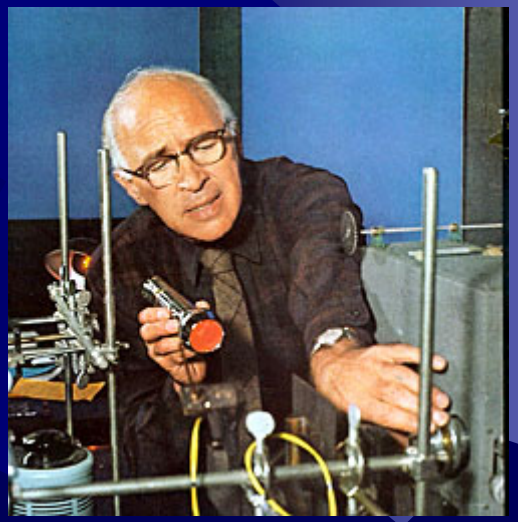
  Information carrying capacity very large

- *Minerals cannot carry the information that biopolymers contain*



Is time the answer?

"*However improbable we regard this event, it will almost certainly happen at least once…. The time… is of the order of two billion years…. Given so much time, the "impossible" becomes possible, the possible probable, and the probable virtually certain. One only has to wait: time itself performs the miracles*." George Wald, in 'The Origin of Life', *Scientific American* (Aug 1964),



What can we expect over the course of time?

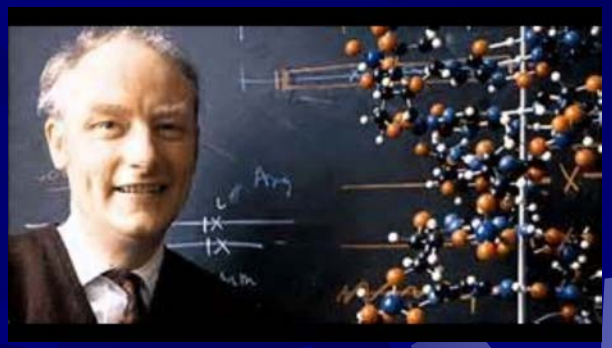
- Over the history of the universe, *is there enough time for life to form by random interactions?*
- *What is the maximum number of "events" (particle interactions) that could have occurred throughout the history of the universe?*
- ~10^{80} elementary particles in
- ~10^{16} sec
- Th
- Ma
- ~10^{43} event
- Probability of one 150 amino acid prot by chance = (probability of incorporating only left-handed amino acids)*(probability of correct amino acid sequencing at every 15th position) =(~10^{-45})*(~10^{-13}) = ~10^{-58}.
- A minimally complex cell requires ~250 proteins. Probability = ~(10^{-58})^{250} = ~$10^{-14,500}$.
- ~$10^{14,250}$ random interactions required to make a cell.

Minimum number of physical interactions to generate a cell by accident = ~$10^{14,250}$

Maximum number of physical interactions since the start of the universe = ~10^{139}

Some honest confessions….

"An honest man, armed with all the knowledge available to us now, could only state that in some sense, the origin of life appears at the moment to be almost a miracle, so many are the conditions which would have had to have been satisfied to get it going."
Francis Crick, Life Itself: Its Origin and Nature (1981)



"The complexity of the simplest known type of cell is so great that it is impossible to accept that such an object could have been thrown together suddenly by some kind of freakish, vastly improbable, event. Such an occurrence would be indistinguishable from a miracle."
Michael Denton, Evolution, A Theory in Crisis (1985)

What does "miracle" mean in the context of origins?

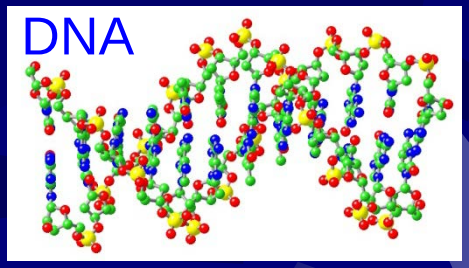
That life was the result of an intelligent mind rather than unguided processes.

Can we test for intelligent design of an origins event?

Can we objectively test for design?

Design in sequences

a string of letters	numbers	molecules
my dog has fleas	3948250	



Criteria for design in a sequence* –

1. High degree of complexity
   → low probability of formation
2. High degree of specificity
   → identifiable by means of a pre-existing pattern
   → communicates specific information

the design test

Example – dyhsfaesmolga
mydoghasfleas

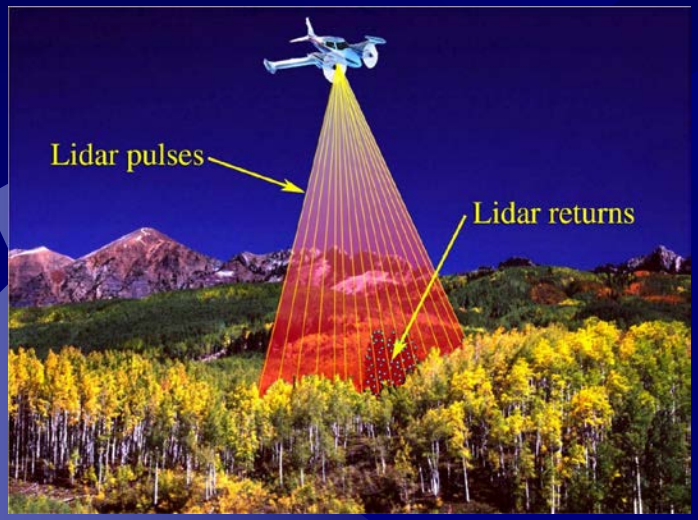
$P = (1/26)^{13} = 4 \times 10^{-19}$

*W.A. Dembski

1. The Design Inference, Cambridge University Press, 1998

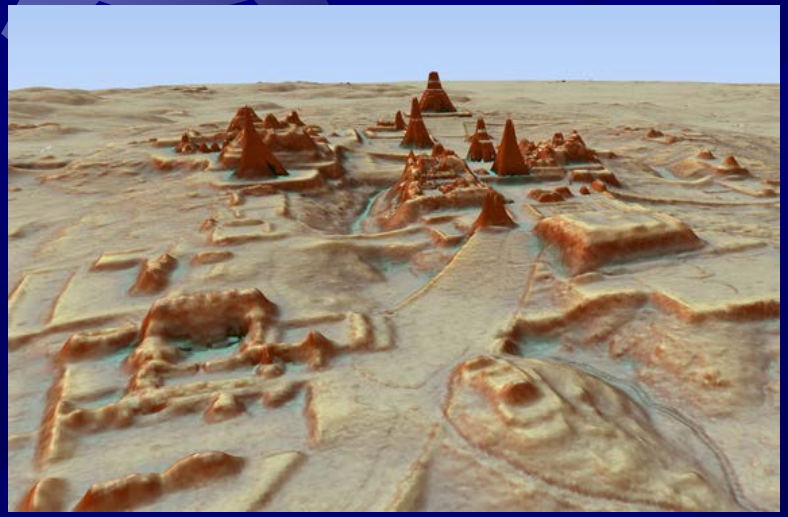
2. Intelligent Design – The Bridge Between Science & Theology, InterVarsity Press,1999

Example – archaeology with LiDAR (Light Detection And Ranging)



60,000 ancient Mayan structures under dense forest in Guatemala

The city of Tikal



T. Clynes, National Geographic, Feb. 1, 2018

Whose paper is whose?

→ 1

→ 0

Which is more likely to be the result of the actual 100 coin flips (i.e. truly random)?

01011011001101001001011010100110010110100110010101
11010101100110101000101100011010110111010101011101

This sequence changes more often than typically occurs in a random coin toss

$P = (1/2)^{100} \sim 10^{-30}$ for both

01000110110000010100111001011011100000010010001101000101011001111000100110100110111010111101111

Very high degree of specificity!

Could the seemingly random sequence have been designed?

2^n where n = 3 2 1 0

			0	0
			1	1
		0	0	0
		0	1	1
		1	0	2
		1	1	3
	0	0	0	0
	0	0	1	1
	0	1	0	2
	0	1	1	3
	1	0	0	4
	1	0	1	5
	1	1	0	6
	1	1	1	7
0	0	0	0	0
0	0	0	1	1
0	0	1	0	2
0	0	1	1	3
0	1	0	0	4
0	1	0	1	5
0	1	1	0	6
0	1	1	1	7
1	0	0	0	8
1	0	0	1	9
1	0	1	0	10
1	0	1	1	11
1	1	0	0	12
1	1	0	1	13
1	1	1	0	14
1	1	1	1	15

False negatives and false positives

False negative – concluding that a sequence does *not* have an intelligent source when in fact it *does*

False positive – concluding that a sequence *does* have an intelligent source when in fact it does *not*

The design test can generate false negatives

The design test typically does not generate false positives

If we find a high degree of specificity, chances are very good that the sequence was designed by an intelligent agent

To falsify the design hypothesis

Demonstrate that an ultra-high information system, at the level of a cell, can originate in a finite amount of time through accidental combinations of the letters used in the language of the system.

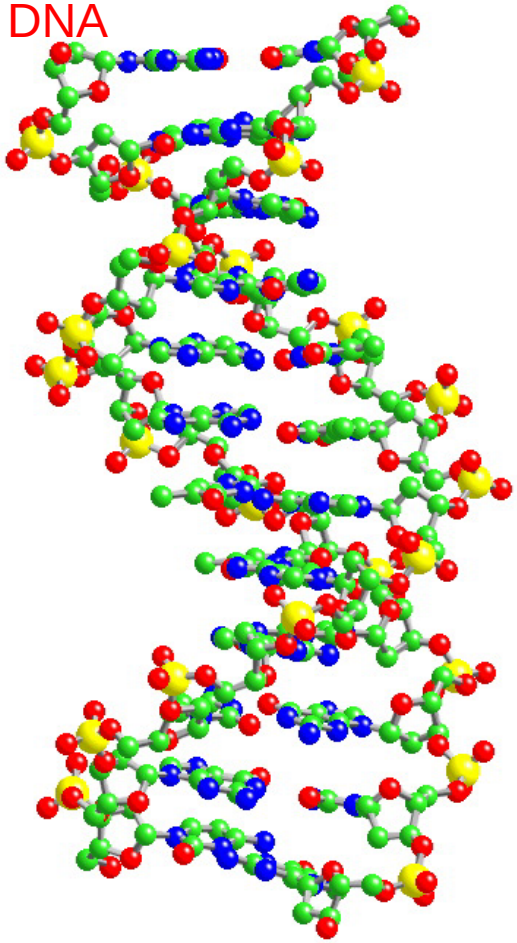
How long?

At one "shake' every second, you have 50:50 odds of success after…
~10^{43} years

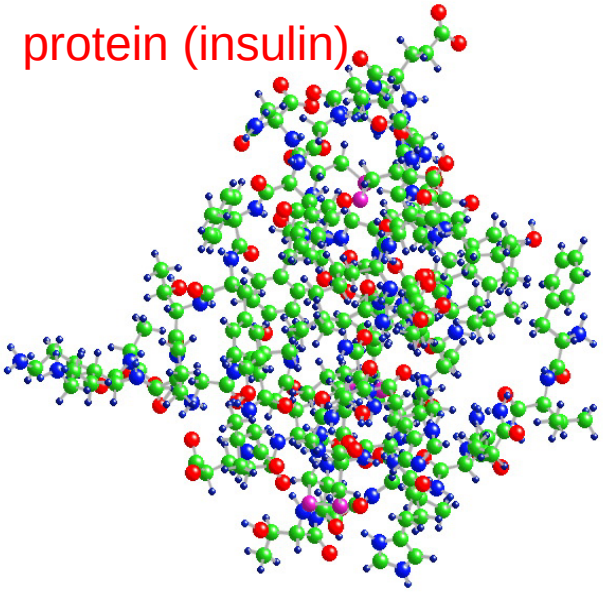
Do biopolymers pass the design test?

- *Are they complex?*
- *Do they exhibit a high degree of specificity?*

DNA



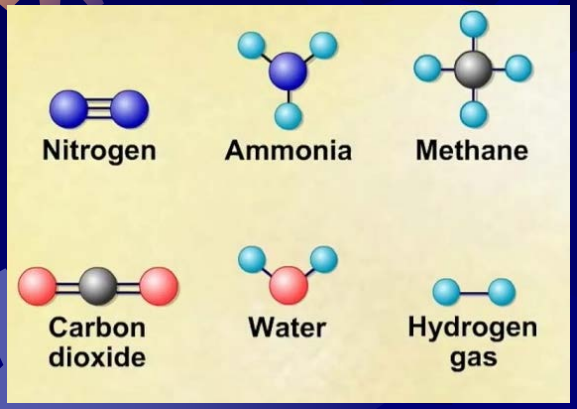
protein (insulin)



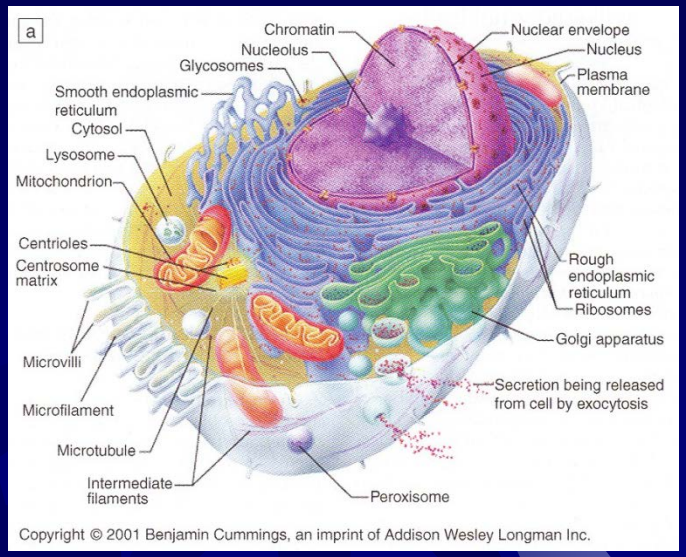
2nd base in codon

1st base in codon	U	C	A	G	3rd base in codon
U	Phe	Ser	Tyr	Cys	U
	Phe	Ser	Tyr	Cys	C
	Leu	Ser	STOP	STOP	A
	Leu	Ser	STOP	Trp	G
C	Leu	Pro	His	Arg	U
	Leu	Pro	His	Arg	C
	Leu	Pro	Gln	Arg	A
	Leu	Pro	Gln	Arg	G
A	Ile	Thr	Asn	Ser	U
	Ile	Thr	Asn	Ser	C
	Ile	Thr	Lys	Arg	A
	Met	Thr	Lys	Arg	G
G	Val	Ala	Asp	Gly	U
	Val	Ala	Asp	Gly	C
	Val	Ala	Glu	Gly	A
	Val	Ala	Glu	Gly	G

Summary



How?



Requirements:

- Highly controlled conditions
- Precise free energy inputs
- Specific sequencing (genetic information)

Inadequate causes:

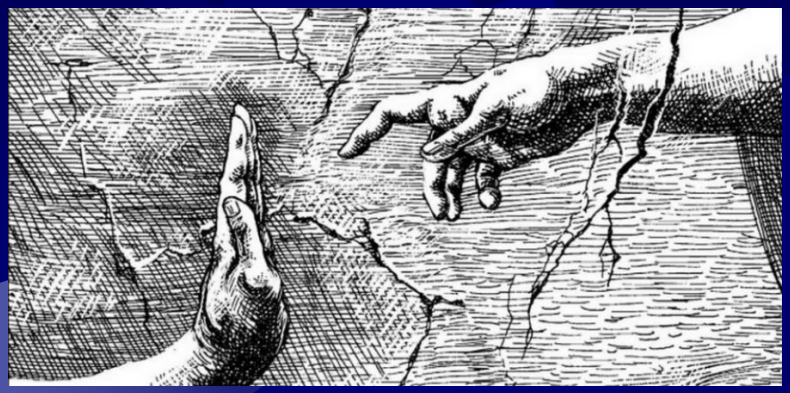
- Undirected energy added to a stew of molecules
- Crystalline minerals
- Time

A reasonable conclusion:

- Life is the result of intelligent design
- *The best explanations for past events typically cite causes that are known from present experience to be capable of producing the effect in question* (Method of multiple competing hypotheses – described by Lyell & Darwin)

EXTRAS

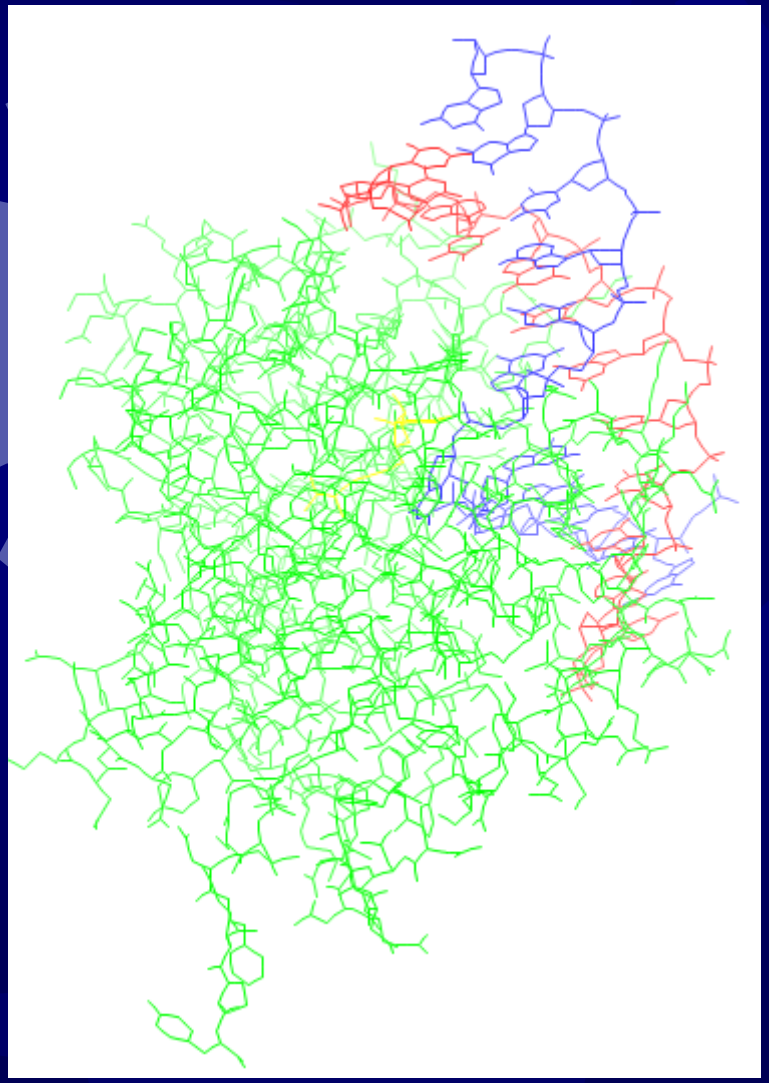
Summary (world view)

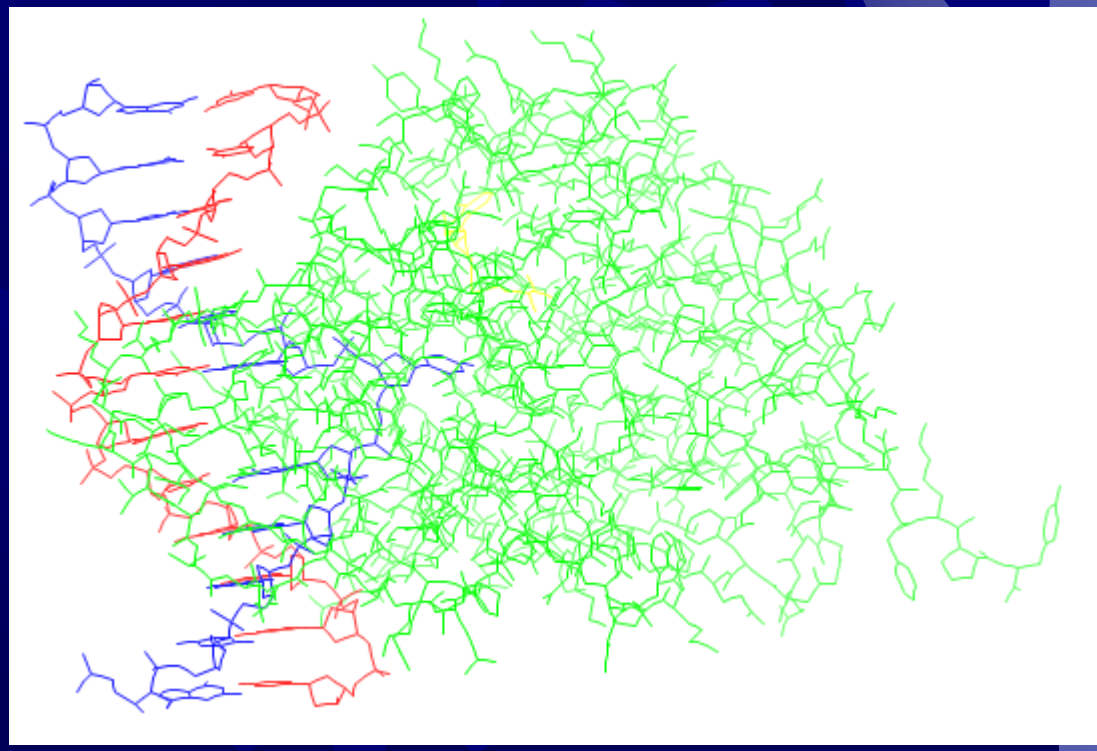


?

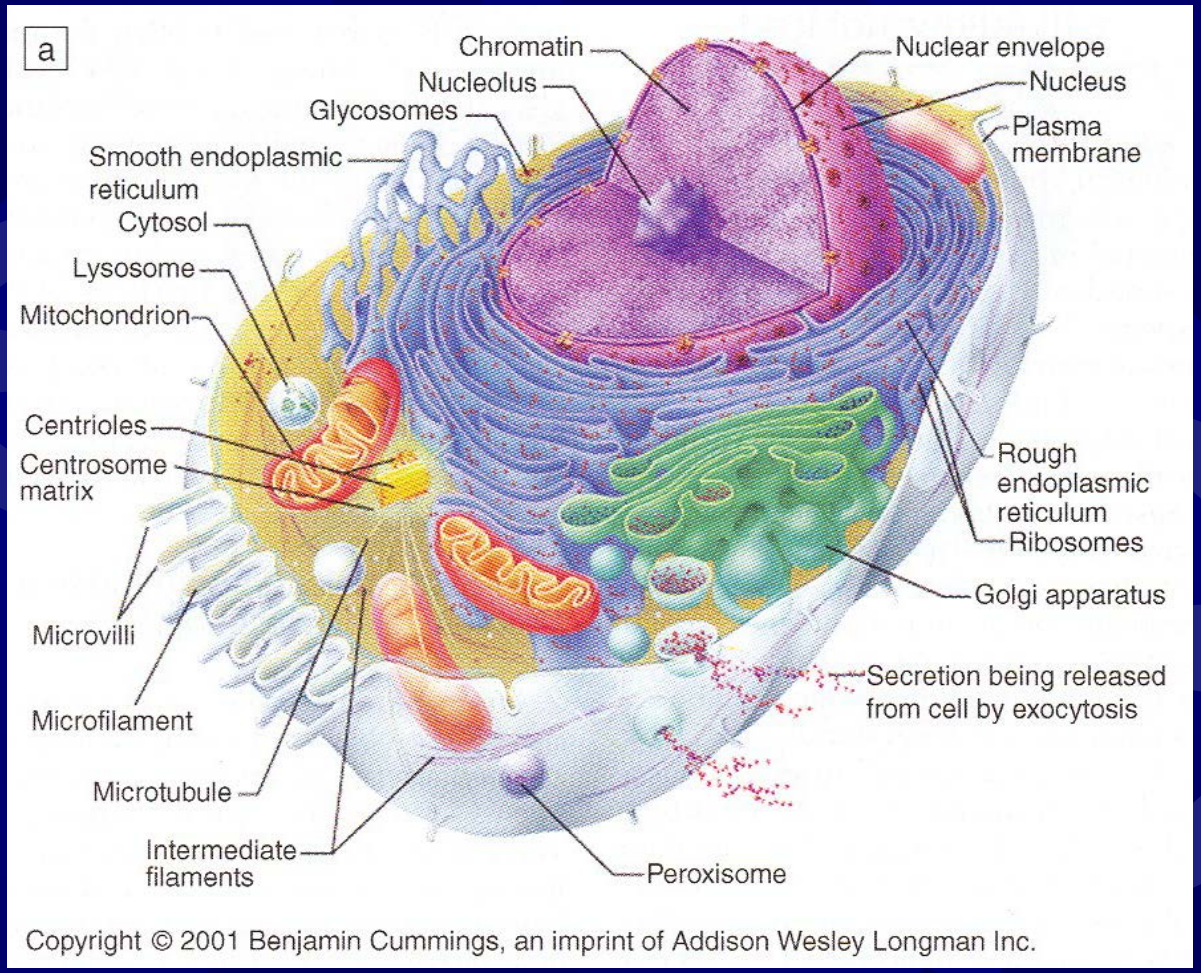
- Your conclusions about the origin of life affect your world view in a big way.
- Implications of a materialist conclusion:
  1. Life is an accident and, therefore, I am an accident.
  2. The only “meaning” to life is what I invent for myself.
- Implications of a design conclusion:
  1. Life presumably has purpose (tied to the purposes of the designer).
  2. We as individuals have purpose.
  3. Meaningful living happens as we discover our purpose in a designed world.
- *Think carefully about this – it will affect the way you think about everything else.*

Protein-nucleic acid interactions – *nanoscience at its best!*





Cells – nested hierarchies of irreducible complexity



*S.C. Meyer, Proc. Biol. Soc. WA. **117**, 213 (2004)*

Example – “geoglyphs”

Watling *et al.*, PNAS **114**, 1868 (2017)

How did we get to where we are today?

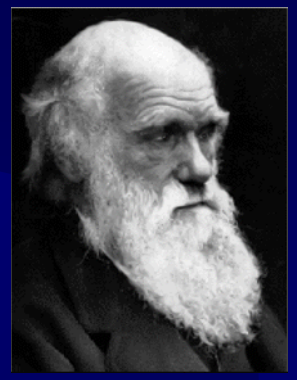
Belief in a designed universe guided the development of modern science

Johannes Kepler (1571-1630) – *celestial mechanics, astronomy*
Blaise Pascal (1623-1662) – *hydrostatics*
Robert Boyle (1627-1691) – *gas dynamics, chemistry*
Nicolaus Steno (1638-1687) -- *stratigraphy*
Issac Newton (1642-1727) – *calculus, mechanics, dynamics*
Michael Faraday (1791-1867) – *magnetism*
Louis Agassiz (1807-1873) – *glacial geology*
James Simpson (1811-1870) -- *gynecology*
Gregor Mendel (1822-1884) – *genetics*
Louis Pasteur (1822-1895) – *bacteriology*
William Thompson -- Lord Kelvin (1824-1907) – *thermodynamics*
Joseph Lister (1827-1912) – *antiseptic surgery*
James Clerk Maxwell (1831-1879) – *electricity and magnetism, statistical thermodynamics*
Carolus Linnaeus (1707-1778) – *modern biological classification*

William Paley – *Natural Theology* (1802)

Basic idea – A watch requires a watchmaker
→ design in nature requires a designer

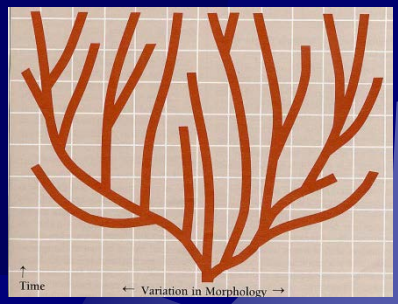
Historical context



Charles Darwin – *The Origin of Species* (1859)

Basic ideas –

- Change → natural selection → microevolution (small changes)
- Extrapolation of microevolution → macroevolution (large changes)
- All existing species evolved from the "originals"
- Cells and biological subsystems *(e.g. vision)* are simple



Neo-Darwinism (1st half of 20th century) = Darwinism + genetics + paleontology + anatomy + embyrology + …

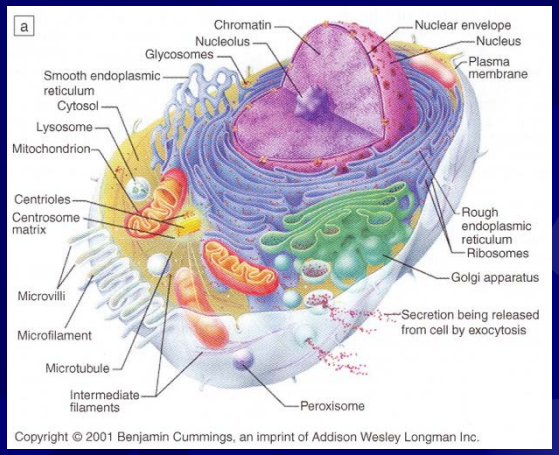
Basic ideas –

- Mutations give rise to small changes that are selected if they give reproductive advantage
- *No limit to the extent of biological change possible*
- Small changes accumulate over time, leading to large changes
- Biological complexity can arise spontaneously - *no design required*

Historical context

Modern biochemistry & molecular biology (2nd half of 20th century on…)

- "Inner workings" of life at a molecular level
- Complexity and efficiency of cells and biological subsystems
- Standard cell equipment:
  - sensors
  - pumps
  - power plants
  - recycling units
  - molecular monorails



"The entire cell can be viewed as a factory that contains an elaborate network of interlocking assembly lines, each of which is composed of a set of large protein machines"

Bruce Alberts, Past President -- National Academy of Science

A materialist perspective

"We take the side of science in spite of the absurdity of some of its constructs, because we have an a priori commitment to materialism. It is not that the methods and institutions of science somehow compel us to accept a material explanation, but, we are forced by our a priori adherence to material causes. Moreover, materialism is absolute, for we cannot allow a Divine Foot in the door."

Richard Lewontin -- Professor Emeritus of Biology, Harvard University

A theistic perspective

"The vast mysteries of the universe should only confirm our belief in the certainty of its Creator. I find it as difficult to understand a scientist who does not acknowledge the presence of a superior rationality behind the existence of the universe as it is to comprehend a theologian who would deny the advances of science."

Werner von Braun --

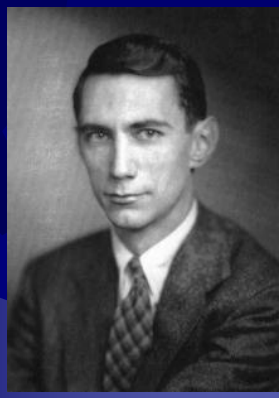
Aerospace engineer

Jonathan D. Eisenback	Professor of Plant Pathology Dept. of Plant Pathology and Weed Science	Virginia Tech
Eduardo Arroyo	Professor of Forensics (Ph.D. Biology)	Complutense University (Spain)
Peter Silley	Ph.D. Microbial Biochemistry	University of Newcastle upon Tyne
E. Norbert Smith	Ph.D. Zoology	Texas Tech University
Peter C. Iwen	Professor of Pathology and Microbiology	University of Nebraska Medical Center
Paul Roschke	A.P. and Florence Wiley Professor, Dept. of Civil Engineering	Texas A&M University
Luman R. Wing	Associate Professor of Biology	Azusa Pacific University
Edward F. Blick	Ph.D. Engineering Science	University of Oklahoma
Wesley M. Taylor	Former Chairman of the Division of Primate Medicine & Surgery	New England Regional Primate Research Center, Harvard Medical School
Don England	Professor Emeritus of Chemistry	Harding University
Wayne Linn	Professor Emeritus of Biology	Southern Oregon University
James Gundlach	Associate Professor of Physics	John A. Logan College
Guillermo Gonzalez	Associate Professor of Astronomy	Iowa State University
Tim Droubay	Ph.D. Physics	University of Wisconsin-Milwaukee
Gregory D. Bossart	Director and Head of Pathology	Harbor Branch Oceanographic Institution
Barry Homer	Ph.D. Mathematics	Southampton University (UK)
Jiøí Vácha	Professor Emeritus of Pathological Physiology	Institute of Pathophysiology, Masaryk University (Czech Republic)
Richard J. Neves	Professor of Fisheries, Dept. of Fisheries and Wildlife Sciences	Virginia Tech
David Deming	Associate Professor of Geosciences	University of Oklahoma
Gregory A. Ator	Associate Professor, Department of Otolaryngology	University of Kansas Medical Center
Erkki Jokisalo	Ph.D. Social Pharmacy	University of Kuopio (Finland)
John S. Roden	Associate Professor of Biology	Southern Oregon University
Donald W. Russell	Adjunct Assistant Clinical Professor	University of North Carolina School of Medicine
Neil Armitage	Associate Professor of Civil Engineering	University of Cape Town (South Africa)
Geoff Barnard	Senior Research Scientist, Department of Veterinary Medicine	University of Cambridge (UK)
Richard Hassing	Ph.D. Theoretical Physics	Cornell University
Olivia Torres	Professor-Researcher (Human Genetics)	Autonomous University of Guadalajara (Mexico)
Donald A. Kangas	Professor of Biology	Truman State University
Alvin Masarira	Senior Lecturer for Structural Engineering and Mechanics	University of Cape Town (South Africa)
George A. Ekama	Professor, Water Quality Engineering, Dept of Civil Engineering	University of Cape Town (South Africa)
Alistair Donald	Ph.D. Environmental Science/Quaternary or Pleistocene Palynology	University of Wales (UK)
Thomas C. Majerus	PharmD; FCCP	University of Minnesota
Ferenc Farkas	Ph.D. Applied Chemical Sciences	Technical University of Budapest (Hungary)
Scott A. Chambers	Affiliate Professor of Chemistry and Materials Science & Engineering	University of Washington
Cris Eberle	Ph.D. Nuclear Engineering	Purdue University
Dennis M. Sullivan	Professor of Biology and Bioethics	Cedarville University
Rodney M. Rutland	Department Head & Associate Professor of Kinesiology	Anderson University
Alastair M. Noble	Ph.D. Chemistry	University of Glasgow (Scotland)
Robert D. Orr	Professor of Family Medicine	University of Vermont College of Medicine
Laverne Miller	Clinical Associate Professor of Family Medicine	Medical College of Ohio
Laura Burke	Former Associate Professor of Industrial Engineering	Lehigh University
Terry W. Spencer	Former Chair, Department of Geology & Geophysics	Texas A&M University
Bert Massie	Ph.D. Physics	University of California, Los Angeles

Information, complexity & intelligence

Basic concepts (from information theory – Claude Shannon)

1. The Shannon information entropy ($S = \ln\Omega$) in a sequence is directly related to the probability of formation and the information content



For a binary sequence *s* (e.g. *s* = 010000110)

I(s) = information content, *p(s)* = probability of formation

$I(s) = -\log_2 p(s)$

Example – *s* = 010000110

$p(s) = (1/2)^9 = 0.00195$

$I(s) = -\log_2(0.00195) = 9$

Information content goes up as probability for formation goes down

2. Information with a high degree of specificity is most likely the result of intelligence

Example – dyhsfaesmolga

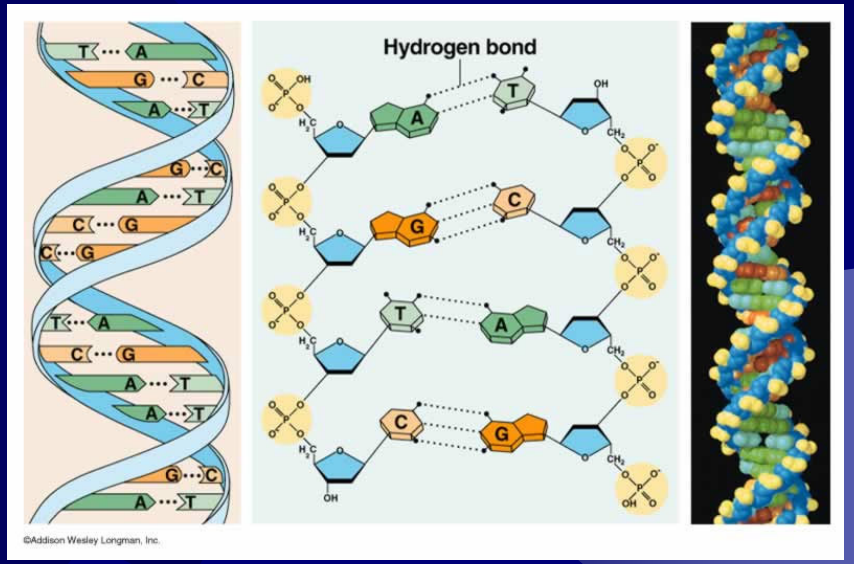
mydoghasfleas -- my dog has fleas

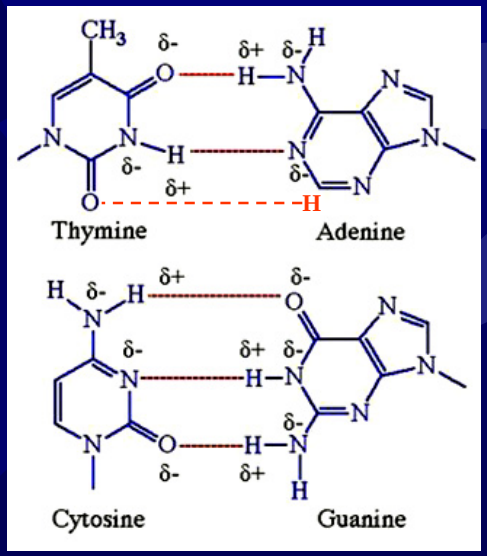
- Same probability of formation
- Same information content
- Only one has specificity (i.e. identifiable by the pattern of the English language) and communicates information

A design feature - built-in error detection in DNA

- 16 possible bases for DNA - Why A, T, G, and C?
- *Hypothesis* -- to minimize transmission errors*
- Connection to error coding theory**
  - Parity bits added to detect errors in bit strings
  - Add a 1 (O) to an odd (even) bit string so the sum of digits is always even
    - e.g. (100110,1) → 4 & (100001,0) → 2
  - *Rationale* – transmission errors: 0 → 1 or 1 → 0
  - *Odd bit sum → error*
  - Represent A, G, T & C as four-bit strings
  - First three: 1 or 0 if H-bonding sites are proton donors (1) or acceptors (0)
  - Fourth: 1 or 0 if base is monocyclic (1) or bicyclic (0)
  - Sum of digits is even for all 4 bases (even parity)
  - A – T & G – C cross bonding → stable DNA
  - If other bases which don't meet these criteria were in DNA → weak bonds → unstable DNA

Characteristic of a carefully designed system





T – (010*,1)
A – (101*,0)
C – (100,1)
G – (011,0)
*Artificial – no actual H bond present here

*Mac Dónaill, Chem Comm 2062-2063 (2002)
Hamming, Bell Syst Tech J **26, 147 (1950)

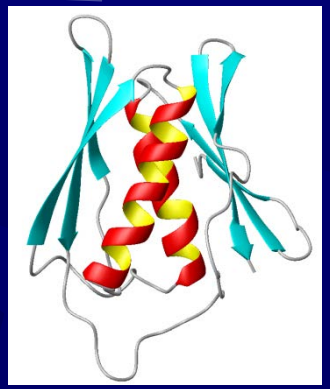
An amino acid set that maximizes biological function

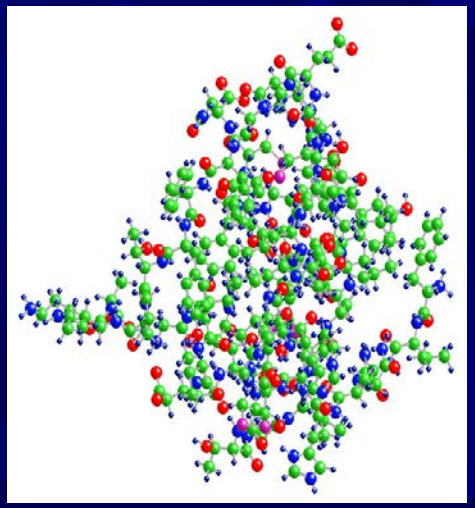
- *50 plausible amino acids on which life could have been built*
- *Huge number of possible combinations (50×49×48×… ×33×32×31 = ~1 × 10^{32})*
- *Why are biological proteins based on the particular set of 20 amino acids we find?*

*Philip & Freeland, "Did Evolution Select a Nonrandom Alphabet of Amino Acids?" Astrobiology **11**, 235 (2011)*

Tested 1 million other combinations of 20 amino acids drawn randomly from the set of 50 and compared each with the actual set on which life is based…

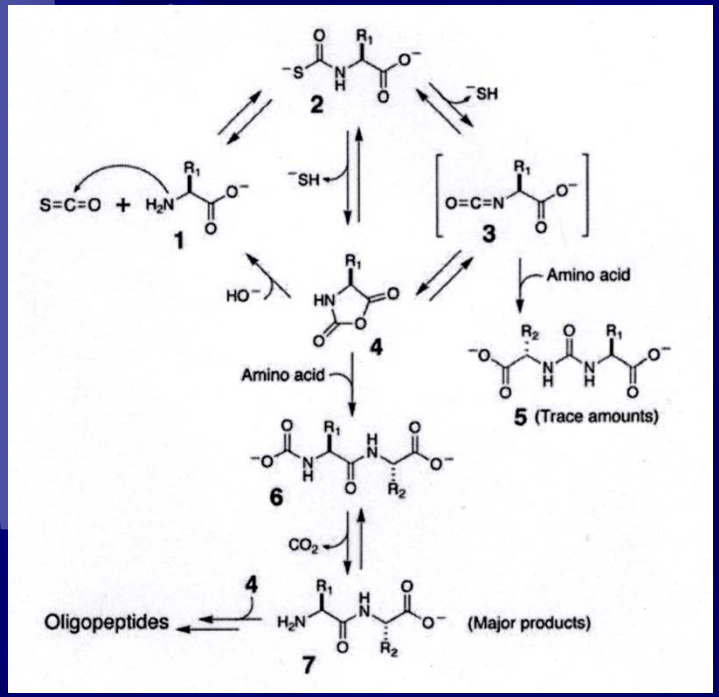
"...the standard alphabet exhibits better coverage (i.e., greater breadth and greater evenness) than any random set for each of size, charge, and hydrophobicity, and for all combinations thereof."



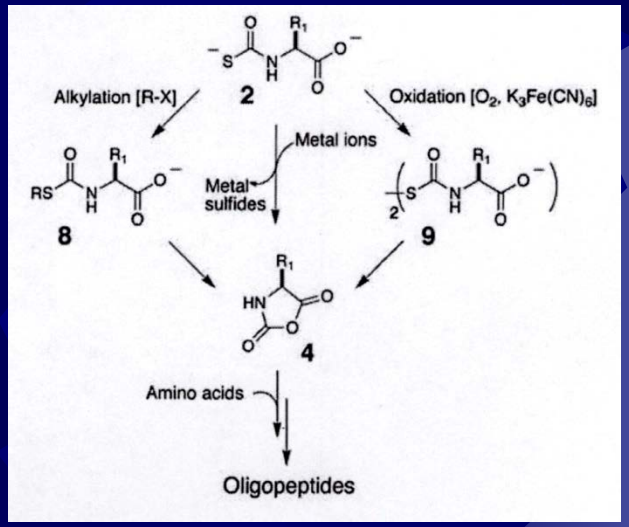


Experimental yields

Carbonyl sulfide (COS -- a volcanic gas) mediates polypeptide in aqueous medium



The rate limiting step (intramolecular cyclization (2 → 4) is catalyzed by metal ions (Fe^{+2}), oxidants & alkylating agents



Limited tripeptide formation from *L*-amino acids over the course of hours

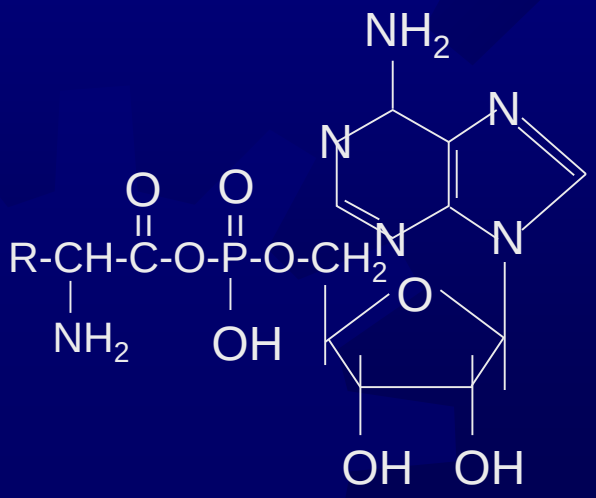
Leman *et al.*, *Science* **306**, 283 (2004)

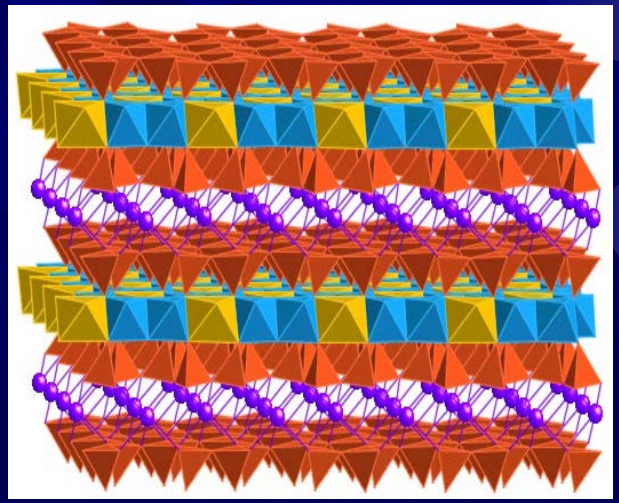
Complexity (information) from an (ordered) crystalline surface?

- Aminoacyl adenylates + montmorillonite clays → polypeptides (~50 units)
  - *Reactants were energy rich (to overcome the free energy barrier)
  - *The clay concentrated the monomers (between layers)
  - *No yield when amino acids were used (no free energy from clay)
  - *Random sequences only

Aperiodic sequencing cannot come from a periodic crystalline surface

- *Complex, specified information in biopolymers must have some other source
- *Configurational entropy work must be done (to overcome chance)
- *Was intelligence involved in the origin of biological polymers?*





Could random interactions over time produce even one cell?

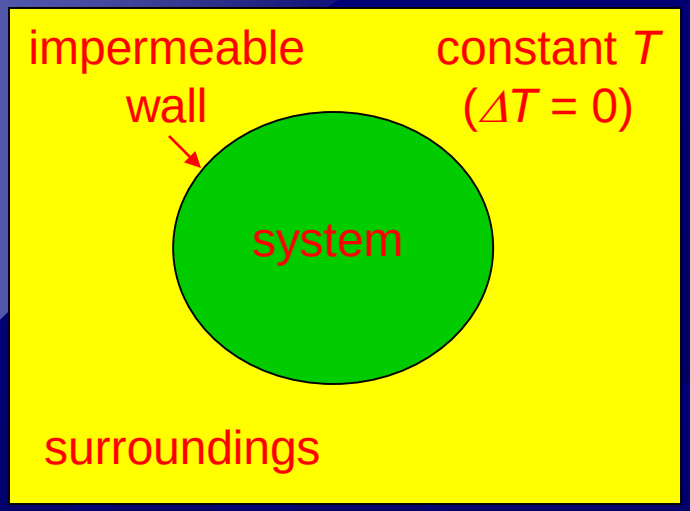
- In a prebiotic universe, would there be enough opportunities for atoms, ions and small molecules to knock around together and form life (without intelligent manipulation)?
- What is the maximum number of "events" (material interactions) that could have occurred throughout the history of the universe?
- ~10^{80} elementary particles in universe. 10^{16} seconds have elapsed since the Big Bang.
- The fastest possible "event" would last as long as it takes for light to travel across the shortest distance over which a physical interaction can take place.
- Shortest distance = Planck length (10^{-33} cm).
- Fastest event would last ~10^{-33} cm/10^{10} cm-sec^{-1} = ~10^{-43} sec.
- Maximum possible number of events since the start of the universe =
- ~10^{43} events-sec^{-1} x 10^{16} sec x 10^{80} particles = ~10^{139}.
- Probability of just one 150 AA protein by chance = (probability of incorporating only left-handed AA)*(probability of correct AA sequencing at every 15th position) =(~10^{-45})*(~10^{-13}) = ~10^{-58}.
- A minimally complex cell requires ~250 proteins. Probability = ~(10^{-58})^{250} = ~$10^{-14,500}$.
- ~$10^{14,500}$ random interactions required to make a cell.
- *Greatly exceeds the maximum possible number of interactions since the universe started…*

Another candid response…

“There are only two possible explanations as to how life arose: spontaneous generation arising to evolution, or a supernatural creative act of God. . . there is no other possibility. Spontaneous generation was scientifically disproved 120 years ago by Louis Pasteur and others, but that leaves us with only one other possibility . . . that life came as a supernatural act of creation by God, but I can't accept that philosophically because I do not want to believe in God. Therefore I choose to believe in that which I know is scientifically impossible, spontaneous generation leading to evolution.”

George Wald, Nobel Prize Winner and Professor Emeritus of Biology at Harvard University

Thermodynamic criteria for spontaneity



- Wall is impermeable to matter, but heat can be exchanged
- Both system and surroundings are in mechanical and thermal equilibrium
- Surroundings in material equilibrium
- System not in material equilibrium

- Mechanical equilibrium:
  1. $\boldsymbol{a}_{cm} = 0$
  2. $\Sigma \boldsymbol{\tau} = 0$
- Thermal equilibrium
  $\Delta T = 0$
- Material equilibrium
  1. Phase – constant amounts of all phases
  2. Reaction – constant amounts of all components

Thermodynamic criteria for spontaneity

For any process within the system,

$dq_{sys} = -dq_{surr}$

$dS_{tot} = dS_{sys} + dS_{surr} \geq 0 \rightarrow dS_{sys} \geq -dS_{surr}$

(2nd law of thermodynamics: > for irreversible processes & = for reversible processes)

$dq_{surr}/T = -dq_{sys}/T$

$dS_{sys} \geq -dS_{surr} = -dq_{surr}/T = dq_{sys}/T$

$dS_{sys} \geq dq_{sys}/T \rightarrow dq_{sys} \leq TdS_{sys}$

Combining with the 1st law of thermodynamics ($dU = dq + dw$),

$dU = dq + dw \leq TdS - PdV$

$dU - TdS + PdV \leq 0$

Thermodynamic criteria for spontaneity

For processes at constant T and P,

$$dU - TdS + PdV \leq 0$$

$$dU + PdV + \cancelto{0}{VdP - VdP} - TdS - \cancelto{0}{SdT + SdT} \leq 0$$

$$dU + PdV + VdP - TdS - SdT \leq 0$$

$$d(U + PV) - d(ST) \leq 0$$

Enthalpy (H) defined as $U + PV$

$$dH - d(ST) = d(H - TS) \leq 0$$

Gibbs free energy (G) defined as $H - TS$

$$d(G)_{T,P} \leq 0$$

Thermodynamic criteria for spontaneity

For processes at constant T and V,

$$dU - TdS + PdV \leq 0$$

$$dU - TdS - SdT + SdT^{0} + PdV^{0} \leq 0$$

$$dU - d(TS) \leq 0$$

$$d(U - TS) \leq 0$$

Helmholtz free energy (A) defined as $U - TS$

$$(dA)_{T,V} \leq 0$$

Physical significance of A:
$-\Delta A$ = maximum possible work available from a system in an isothermal process

Thermodynamic criteria for spontaneity

Physical significance of *A*:

$$dU - TdS + PdV \leq 0$$

$$dU - TdS - dw \leq 0$$

$$dU - TdS - SdT + SdT - dw \leq 0$$

$$d(U - TS) \leq -SdT + dw$$

$$dA \leq -SdT + dw$$

At constant T,

$$dA \leq dw$$ (work done *on* the system)

$$dA \leq -dw$$ (work done *by* the system)

$$-dA \geq dw$$

$-\Delta A$ = maximum possible work available from a system in an isothermal process at constant volume

Thermodynamic criteria for spontaneity

Physical significance of *G*:

$dU - TdS + PdV \leq 0$

$dU - TdS - dw \leq 0$

$dU + PdV - PdV + VdP - VdP - TdS - SdT + SdT - dw \leq 0$

$d(U + PV) - d(TS) - PdV - VdP + SdT - dw \leq 0$

$dG - PdV - VdP + SdT - dw \leq 0 \quad (dw = dw_{nonPV} + PdV)$

At constant P & T,

$dG \leq dw_{nonPV} + PdV + PdV$ (work done *on* the system)

$dG \leq -dw_{nonPV} - PdV + PdV$ (work done *by* the system)

$-dG \geq dw_{nonPV}$

$-\Delta G$ = maximum possible non-*PV* work available from a system in an isothermal process at constant pressure

The energetics of biopolymer formation

Thermodynamic criteria for “spontaneity” (a process spontaneously going forward)

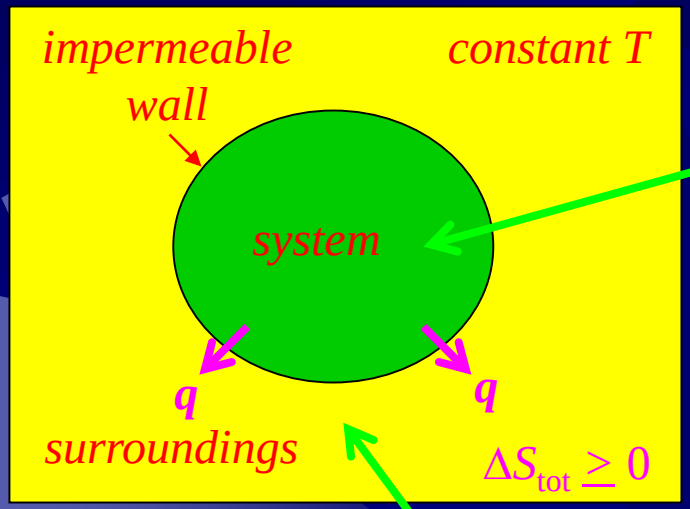
For any process in a closed system,

$$\Delta S_{tot} \geq 0$$

For any process in an open system at constant T & P,

$$(\Delta G)_{T,P} \leq 0$$

Spontaneous crystallization of ice below the freezing point of water



$H_2O_{(l)}$ (-10°C) → $H_2O_{(s)}$ (-10°C)

A reversible path…. (T_1 = -10°C, T_2 = 0°C)

$H_2O_{(l)}$ (T_1) → $H_2O_{(l)}$ (T_2) $\Delta S = C_l \ln(T_2/T_1) = 0.67$

$H_2O_{(l)}$ (T_2) → $H_2O_{(s)}$ (T_2) $\Delta S = \Delta H_{fus}/T_2 = -5.26$

$H_2O_{(s)}$ (T_2) → $H_2O_{(s)}$ (T_1) $\Delta S = C_s \ln(T_1/T_2) = -0.33$

$H_2O_{(l)}$ (-10°C) → $H_2O_{(s)}$ (-10°C) ΔS_{sys} = -4.92 Cal/mol-K

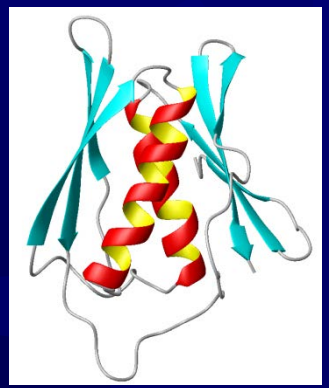
$\Delta S_{surr} = q/T_1 = \Delta H_{fus}/T_1$ = +5.11 Cal/mol-K

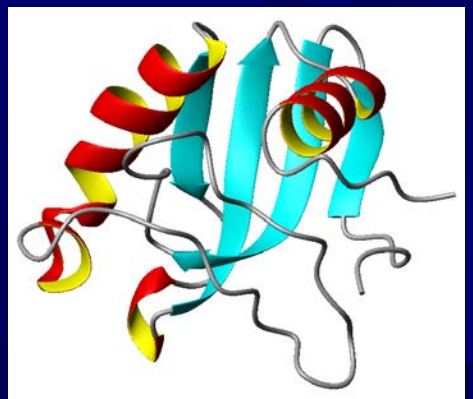
$\Delta S_{tot} = \Delta S_{sys} + \Delta S_{surr}$ = +0.19 Cal/mol-K

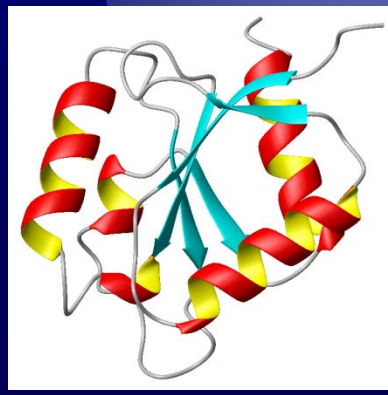
Since ice can spontaneously crystalize from water (order from disorder), can't ordered biopolymers spontaneously form out of disordered biomonomers?

Kinetic realities

- 500 amino acid protein & every 10th is critical to biological function (50 specific amino acids)
- Number of possible configurations = 20^{50} = ~10^{65}
- Synthesize 1000 trial proteins per second for 4.5 billion years
- ~10^{20} total trial proteins made in 4.5 billion years
- ~10^{-43} % of all possible configurations at this (high) rate
- *Not nearly enough time in the entire age of the earth to make even one protein by trial and error*
- Mass of 10^{65} proteins = ~10^{43} Kg
- Mass of the earth = 6 x 10^{24} Kg







The origin of life by non-directed chemistry -- a given?

"For those who are studying aspects of the origin of life, the question no longer seems to be whether life could have originated by chemical processes involving non-biological components but, rather, what pathway might have been followed."
—National Academy of Sciences (1996)

"More than 30 years of experimentation on the origin of life in the fields of chemical and molecular evolution have led to a better perception of the immensity of the problem of the origin of life on Earth rather than to its solution. At present all discussions on principal theories and experiments in the field either end in stalemate or in a confession of ignorance."
-- Klaus Dose, "*The origin of life: More questions than answers.*" Interdisciplinary Science Review, 13, 348-356. (1988).

One candid response…

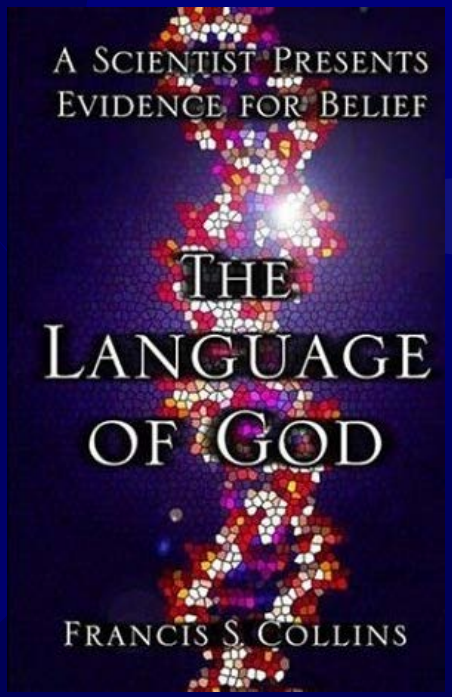
On the appearance of design in biology….

"The almost irresistible force of the analogy (of design) has completely undermined the complacent assumption, prevalent in biological circles over most of the past century, that the design hypothesis can be excluded on the grounds that the notion is fundamentally a metaphysical concept and therefore scientifically unsound. On the contrary, the inference to design is an induction based on a ruthlessly consistent application of the logic of analogy. The conclusion may have religious implications, but it does not depend on religious presuppositions".

Michael Denton, *Evolution: A Theory in Crisis (New Developments in Science are Challenging Orthodox Darwinism)*
Ch. 14, The Puzzle of Perfection, p. 341 (Alder & Alder Publishers, 1986)

From the man who led the effort to elucidate the human genome.....

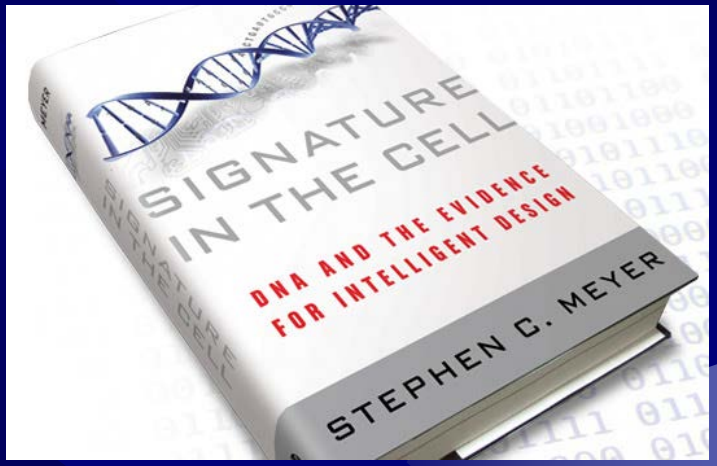
"When you have for the first time in front of you this 3.1 billion-letter instruction book that conveys all kinds of information and all kinds of mystery about humankind, you can't survey that going through page after page without a sense of awe. I can't help but look at those pages and have a vague sense that this is giving me a glimpse of God's mind."
Francis Collins – M.D., Ph.D. & Director, US National Human Genome Research Institute



An insightful perspective….

"Everywhere in our high-tech environment we observe complex events, artifacts, and systems that impel our minds to recognize the activity of other minds: minds that communicate, plan, and design. But to detect the presence of mind, to detect the activity of intelligence in the echo of its effects, requires a mode of reasoning -- indeed, a form of knowledge -- that science, or at least official biology, has long excluded. If living things -- things that we manifestly did not design ourselves -- bear the hallmarks of design, if they exhibit a signature that would lead us to recognize intelligent activity in any other realm of experience, then perhaps it is time to rehabilitate this lost way of knowing and to rekindle our wonder in the intelligibility and design of nature that first inspired the scientific revolution."

Stephen C. Meyer – Director, Center for Science & Culture, Discovery Institute, Seattle, WA



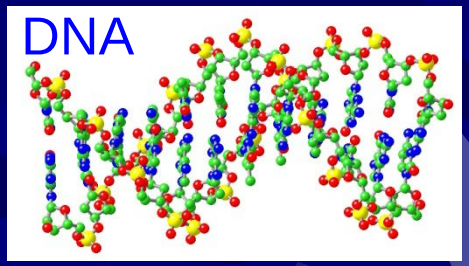
Did crystalline minerals play a role?


CONTACT

The design test

Design in sequences

a string of letters	numbers	molecules
my dog has fleas	3948250	



Criteria for intelligent design of a sequence –

1. High degree of complexity
   → low probability of formation
2. High degree of specificity
   → identifiable by means of a pre-existing pattern
   → communicates specific information

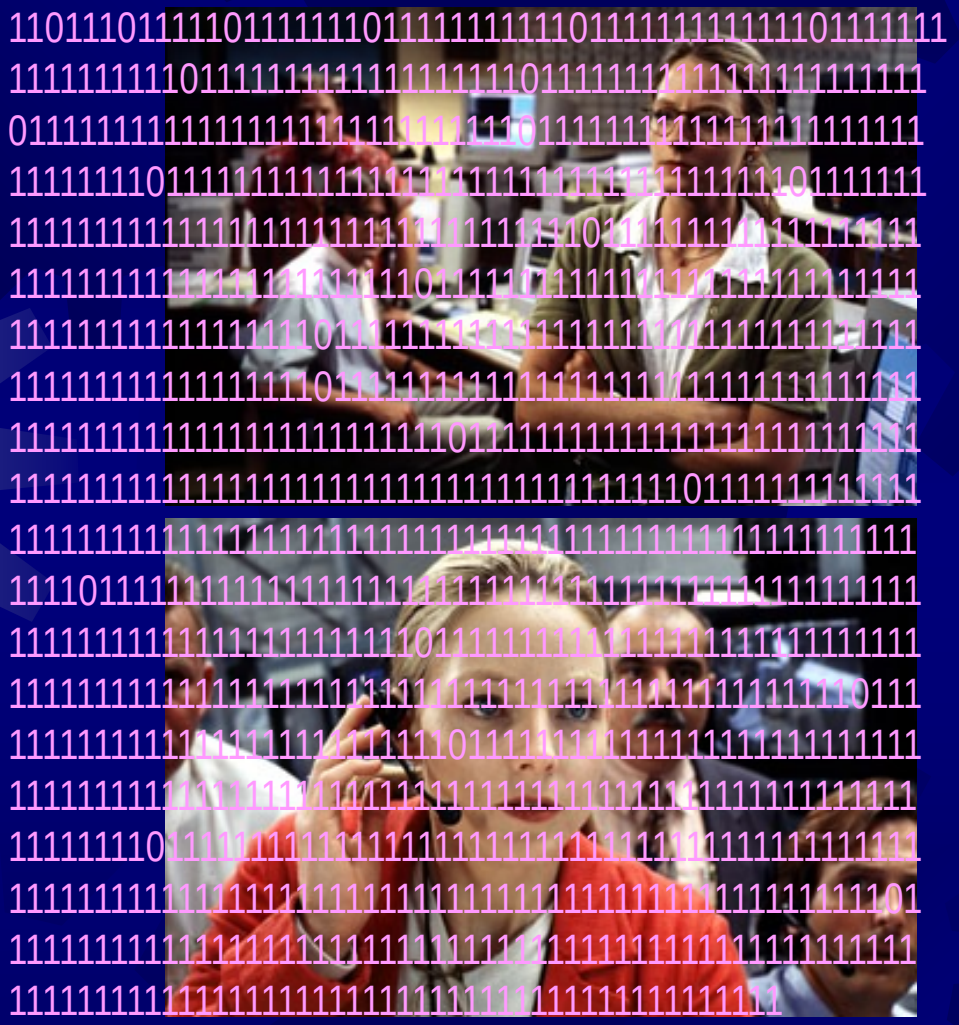
the design test

Example – dyhsfaesmolga
mydoghasfleas

$P = (1/26)^{13} = 4 \times 10^{-19}$

(W.A. Dembski, *The Design Inference*, Cambridge University Press, 1998, and *Intelligent Design – The Bridge Between Science & Theology,* InterVarsity Press,1999)

Did the signal pass the design test?



1072
1’s and 0’s

high degree
of complexity

low probability
of formation

$P = (1/2)^{1072}$
$= \sim 0$

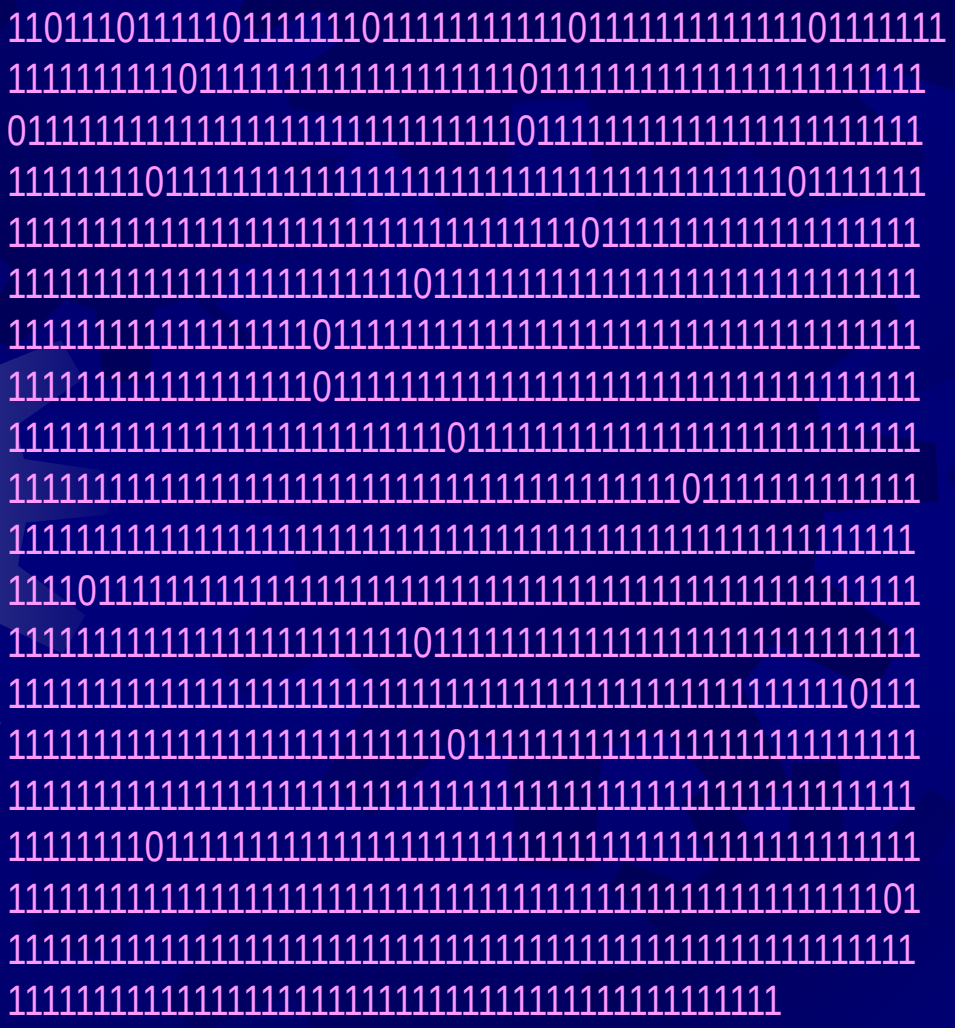
High degree of specificity –
The prime numbers between 2 and 101

False negatives and false positives

False negative – concluding that a sequence does *not* have an intelligent source when in fact it *does*

False positive – concluding that a sequence *does* have an intelligent source when in fact it does *not*

The design test can generate false negatives



1072
1’s and 0’s

high degree
of complexity

low probability
of formation

$P = (1/2)^{1072}$
$= \sim 0$

High degree of specificity –
The prime numbers between 2 and 101 (separated by zeros)

False negatives and false positives

False negative – concluding that a sequence does *not* have an intelligent source when in fact it *does*

False positive – concluding that a sequence *does* have an intelligent source when in fact it does *not*

The design test can generate false negatives

The design test typically does not generate false positives

If we find a high degree of specificity, chances are very good that the sequence was designed by an intelligent agent