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INTERNAL REPORT
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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

Cyril Ponnamperuma Memorial.
Trieste Conference on Chemical Evolution, IV:
Physics of the Origin and Evolution of Life

SUMMARIES*

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Miramare, Trieste (Italy)
4-8 September 1995

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In this Internal Report we have gathered together some of the summaries of the papers to be read at the Conference, which were available at the time of going to press. The meeting was possible thanks to the generous support of the International Centre for Theoretical Physics, the International Centre of Genetic Engineering and Biotechnology, UNESCO, Université Paris 12 - Val de Marne and the European Space Agency.

Julian Chela-Flores
Francois Raulin
Directors

20 August 1995

Abstract for the Trieste Conference on Chemical Evolution IV:
Physics of the Origin and Evolution of Life "Cyril Ponnamperuma Memorial",
Trieste, 4-8 September, 1995.

Ab Initio Calculation of Molecular Energies Including Parity Violating Interactions

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A new approach, RHF-CIS, based on the perturbation of the ground state RHF wave function by the CIS excitations, has been implemented for evaluations of energy of parity violating interaction in molecules, E_{pv}. The earlier approach, RHF-SDE, was based on the perturbation of the RHF ground states by the single-determinant "excitations" (SDE). The results obtained show the dramatic difference between E_{pv} values in the RHF-CIS framework and those in the RHF-SDE framework: the E_{pv} values of the RHF-CIS formalism are more than one order of magnitude greater compared to the RHF-SDE formalism as well as the corresponding tensor components. The maximal *total* value obtained for hydrogen peroxide in the RHF-CIS framework is 3.661×10^{-19} E_H (DZ** basis set) while the maximal E_{pv} value for the RHF-SDE formalism is just 3.635×10^{-20} E_H (TZ basis set). It is remarkable that both in the RHF-CIS and in the RHF-SDE approaches the diagonal tensor components of E_{pv} strictly follow the geometry of a molecule and are always different from zero at chiral conformations. The zeros of the total E_{pv} at chiral geometries are now found to be the results of the interplay between the diagonal tensor components values. We have carried out exhaustive analysis of the RHF-SDE formalism and found that it is not sufficiently accurate for studies of E_{pv}. To this end, we have completely reproduced the previous work, which has been done in the RHF-SDE framework, and developed it further, studying how the RHF-SDE results vary when changing size and quality of basis sets. This last resource doesn't save the RHF-SDE formalism for evaluations of E_{pv} from the general failure. Packages of FORTRAN routines called ENWEAK/RHFSDE-93 and ENWEAK/RHFCIS-94 have been developed which run on top of an *ab initio* MO package. We used $6-31G$ and $6-31G**$, DZ and $DZ**$, TZ and $TZ**$, and $(10s,6p,**)$ basis sets. We will discuss the importance of the present results for possible measurement of the parity violating energy difference between enantiomers of chiral molecules.

Evolutionary, kinetic and thermodynamic aspects on the bioenergetics of inorganic pyrophosphate (PPi) and adenosine triphosphate (ATP)

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Energy barriers for energy carriers are of fundamental significance for the successful operation of the bioenergetic reactions in living cells. PPi and ATP are outstanding "energy-rich" examples of molecular "energy currencies" in biological systems, with kinetic barriers preventing excessively fast thermodynamically feasible hydrolysis from occurring. The barriers may be considered to facilitate the energy coupling roles of these phosphate compounds, which are to secure growth and maintain numerous other energy requiring functions. The enzymes involved in overcoming the energies of acivation of the bioenergetic reactions have evolved to be very well tuned for their roles.

Three aspects will be discussed in some detail. The first is the fact that ATP at neutral pH is considerably more energy-rich than PPi, which thus has been called a "poor man´s ATP". This is exemplified by the kinetic and thermodynamic differences observed between the requirements for the photosynthetic formation of PPi and ATP in certain photobacterial chromatophores by varying levels of energy supply. At lower pH, PPi and ATP are equally energy-rich, which may be of significance for acidophiles. The second concerns the possible evolutionary significance of the finding that, in the dark, a pH gradient suffices to drive extensive PPi synthesis, whereas ATP synthesis requires both a pH gradient and a membrane potential (Strid *et al*, Biochim. Biophys. Acta 892 (1987) 236-244). Thirdly, PPi as the most plausible predecessor to ATP in the origin and early evolution of life, will be discussed.

SUMMARY

ROLE OF TRANSIENT AND STABLE MOLECULES IN CHEMICAL EVOLUTION

by

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Identification of a large number of transient and stable molecules in space ranging from simple diatomics to fairly complex polyatomic species like cyanopolyenes (HCCCCCCCCCCCN) has provided with a scenario for some exotic physio-chemical events leading to their formation.

The composition of Jupiter and Titan atmospheres and laboratory studies on simulated Jovian, Titan and Primordial Earth atmopheres have revealed the importance of many organic compounds like HCN, CO, C_2H_2 etc., in chemical evolution. The reactivities of molecules like HCN, NH_3, HCHO, C_2H_2 and H_2O etc., in primordial earth experiments leading to the formation of amino acids, nucleic acid bases, sugars and other building blocks necessary for the origin of life, have been well demonstrated. Similarities between products from laboratory experiments and those identified from some meteorites as well as their relationship to molecular species in the interstellar medium give ample support to general concepts of Chemical Evolution.

FIRST STEPS IN EUKARYOGENESIS:
Physical phenomena in the origin and evolution of chromosome structure (*)

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Abstract.

Our present understanding of the origin and evolution of chromosomes differs considerably from current understanding of the origin and evolution of the cell itself. Chromosome origins have been less prominent in research, as the emphasis has not shifted so far appreciably from the phenomenon of primeval nucleic acid encapsulation to that of the origin of gene organization, expression, and regulation. In this work we discuss some reasons why preliminary steps in this direction are being taken. We have been led to examine properties that have contributed to raise the ancestral prokaryotic programmes to a level where we can appreciate in eukaryotes a clear departure from earlier themes in the evolution of the cell from the last common ancestor. We shift our point of view from evolution of cell morphology to the point of view of the genes. In particular, we focus attention on possible physical bases for the way transmission of information has evolved in eukaryotes, namely, the inactivation of whole chromosomes. The special case of the inactivation of the X chromosome in mammals is discussed, paying particular attention to the physical process of the spread of X inactivation in monotremes (platypus and echidna). When experimental data is unavailable some theoretical analysis is possible based on the idea that in certain cases collective phenomena in genetics, rather than chemical detail, are better correlates of complex chemical processes.

(*) *Lecture to be delivered at the **Cyril Ponnamperuma Memorial Conference.** The Fourth Trieste Conference on Chemical Evoluion: Trieste, 4-8 /9/95*

(+) Also at the Instituto Internacional de Estudios Avanzados (Universidad Simon Bolivar). Apartado 17606 Parque Central. Caracas 1015A, Venezuela.

COSMOLOGY: THE UNIVERSE IN EVOLUTION

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Abstract

There are three principal pieces of evidence which, when taken together, support the notion that the Universe as a whole is evolving. These are: (a) the Hubble velocity-distance relationship; (b) the abundance of light elements in the Universe; and (c) the three degree cosmic background radiation. The best explanation of these observations is that the Universe began, if it had a beginning, in a hot dense state and it has been expanding and cooling down ever since. In the course of that process matter came to be out of energy, galaxies and stars formed, and you and I came to exist. In this process the emergence of organic material in general, and human beings in particular, seems to have required a very fine tuning of the evolutionary process itself. We do not yet have a definitive scientific explanation of that fine tuning and, therefore, we do not yet understand the linkage of the human being to cosmic evolution. But some interesting suggestions can be made.

CYRIL PONNAMPERUMA MEMORIAL
TRIESTE CONFERENCE ON CHEMICAL EVOLUTION, IV:
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SETI from the Moon

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In case an extraterrestrial artificial signal is discovered, this will be immediate proof that civilizations are plenty in the cosmos and the odds are that, with our freshly acquired experience, we shall readily unravel a dozen of them within a few years. Then the drive to investigate them, in all of their obligatory varieties, will get quite strong.

Extrapolating the fact that for the last 30 years the efficiency of our SETI detection systems doubled each eight months, a dramatic progression, we shall get access to fainter and fainter extraterrestrial emitters. Unfortunately, the Earth or near-Earth man-made radio interferences will become a stronger and stronger obstacle to these investigations.

It is why I recently proposed that a quite neatly singled-out crater on the far-side of the Moon, crater *Saha*, be declared a dedicated safe zone for SETI for the coming generation. Considering that it is a political and philosophical duty for Humankind to provide for such a unique and limited protected lunar location, I suggested that international planning at the time scale of 20-30 years be started at the level of programmatic, technical and legal issues.

In the words of Ambassador Aldo A.Cocca, Professor of Law at the Buenos Aires Council of Advanced International Studies: "The reservation of a Lunar zone for scientific activities, and its further utilization aiming to the common good of humanity, must be recognized and constitutes a precedent (...) The proposal must be supported with the legal framework it requires."

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Organics in the Solar System:
Laboratory Spectroscopic Data Bases for Remote Sensing

ABSTRACT

Prebiotic chemistry in Earth's atmosphere has been described in the literature in terms of irradiation of gas mixtures with compositions ranging from extreme reducing (similar to that on Titan) and less reducing (somewhat similar to that on Mars).Comets have also been proposed to be among the carriers of the two key molecules, HCN and CH2O. We present results on the infrared spectra of irradiated solid and gas mixtures corresponding to the two extreme compositions. Implications of these results in the light of Voyager IRIS observations of Titan and some Comets will be discussed.

Boltzmann's Dynamics on the Primitive Earth about 3.9 Billion Years Ago

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An evolutionarily significant event that could have happened on the primitive earth would be a process of enhancing energy concentrations locally. Once the concentrated energy be released, it could drive various molecular association and dissociation.

We have examined, both theoretically and experimentally, a possibility of forming such microscopic heat engines feeding upon the then available thermal environment. Theoretically, Boltzmann's dynamics of molecules that would lose their memory of past collisions with others is found to uphold those molecules that could feed upon thermal energy if the thermal environment would fluctuate through, for instance, a diurnal cycle. Experimentally, thermal heterocomplex molecules from amino acids, that could have been ubiquitous on the primitive earth, are shown to carry with themselve a wide variety of quasi-stable states such that they could remain in excited states for a considerable period of time even if the temperature of the thermal environment is lowered. The stored energy in these excited states, once released, can be utilized as a factor for driving various molecular association and dissociation.

Lightning Associated to Archean Volcanic Ash-Gas Clouds*

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Lightning discharges of hundreds of meters in length are frequently generated during volcanic eruptions, in which gases and tephra are emitted simultaneously into the atmosphere. However, there has been little opportunity to investigate such a phenomenon. The studies performed during the eruptions of Surtsey in 1963-1964 and Redoubt in 1990 allow us to gain insights into the origin and nature of volcanic lightning. The energy dissipated by these electric discharges is about 10^6 J flash^{-1}. It is estimated that the lightning flux would be about 10^5 J km^{-2} min^{-1} during the explosive phase of a volcano.

Was volcanic lightning an efficient energy source in the archean for the synthesis of prebiotic molecules? To answer this question, one must know the chemical compositions of the gases emitted by volcanoes as well as that of the atmosphere, due to instant dilution effects. It is now generally accepted that the primitive Earth's atmosphere was composed of carbon dioxide, nitrogen and water vapor. The composition of volcanic gases is, however, a subject for considerable variations due to a heterogeneous mantle from which the volatiles are released. Recent isotopic analyses of noble gases trapped in volcanic glasses suggest that Hawaiian volcanoes originate from a primordial, undegassed reservoir deep in the Earth's mantle. Therefore, the volatiles emitted by Hawaiian volcanoes could, perhaps, exemplify more accurately the nature of gases emitted by archean volcanoes. The typical composition of the gases emitted by the Kilauea during a one-stage degassing process is: H_2O (52.30%), CO_2 (30.87%), SO_2 (14.59%), CO (1.00%), H_2 (0.79%) and H_2S (0.16%), among others. *A priori* it could be inferred that volcanic lightning is advantageous for the synthesis of hydrogen cyanide and formaldehyde, due to the presence of reduced gases within the volcanic ash-gas cloud. However, previous electric discharge experiments have not been done in the presence of significant amounts of water vapor, which could cause an inhibitory effect. Consequently there is a necessity for an experimental evaluation.

We are currently studying the effects of spark discharges through a gas mixture composed of H_2O, CO_2, N_2, CO and H_2 by GC-FTIR-MS. To determine the energy yields of the products formed, we are also measuring the energy delivered by the spark discharge using calorimetric and electric techniques developed in our laboratory. We will present recent progress in this experimental work.

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COSMIC EVOLUTION, LIFE AND MAN

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Abstract

Among the most basic problems confronting science are those regarding the origin of the universe, the origin of life and the origin of man. The first question is being studied by cosmologists and theoretical physicists. Whether there is one, or an infinite number of universes, is not the fundamental question, neither is the sequence of events beginning at "zero time" after the primordial explosion of a hydrogen-helium primeval "miniball". The real question is the reality-status of the universe before "zero time" which theorists say is not within the realm of cosmology. At any rate, given primordial hydrogen, the observational and experimental studies demonstrate that all the biogenic and other elements of the periodic system can be generated by nuclear reactions. After hydrogen, the first nuclide formed is helium, or an alpha particle. The next most important thermonuclear reaction is the, so called, triple alpha process. This process which occurrs in the interior of carbon stars at a temperature of 100 million degrees is responsible for the nuclear formation of carbon. The synthesis of such a remarkable nuclide is a unique event without which we would not be able to talk about life on Earth. This general overview starts (1) with a brief introduction addressed primarily to the Cyril Ponnamperuma Memorial. Then, the thesis is presented that the appearance of life and intelligence on our planet can be understood as the result of a number of cosmic and biological evolutionary processes, including (2) The stellar thermonuclear synthesis of the biogenic elements other than hydrogen (C, N, O, P and S), their dispersal into space, and their combination into circumstellar and interstellar molecules. (3) The formation of the Solar System and the Earth-Moon System (4) The role of comets and carbonaceous chondrites in contibuting organic matter to the primitive Earth. (5) The prebiotic synthesis of amino acids, purines, pyrimidines, fatty acids, and other biochemical monomers. (6) The prebiotic condensation reactions leading to the synthesis of oligomers such as oligonucleotides and oligopeptides, with replicative and catalytic activities. (7) The synthesis of amphiphilic lipids, and their self-assembly into liposomes with bi-layered membranes. (8) The formation of protocellular structures. (9) The activation of protocells into a functioning Darwin's ancestral cell. (10) Early evolution of life. (11) The K-T boundary event and the disappearance of dinosaurs. (12) Evolution of hominids leading to *Homo sapiens*. (13) The rapid development of civilization. (14) The exploration of the Solar System. (15) Life beyond our planetary system. (16) Epilogue. Peace from cosmic evolution?

Biosynthesis of Membrane Lipids of Thermophilic Archaebacteria and its Implication to Early Evolution of Life

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The unit lipid of cell membranes of archaebacteria is unique ether lipids, O-dialkylated glycerol with a polar head group at sn-1 position. The chirality of glycerol moiety of the lipids is opposite to that of other kingdoms. The hydrophobic portion consists of saturated C_{20} isoprenoid hydrocarbon backbone and is connected to glycerol by an ether linkage. In addition, cell membranes of some of thermophilic archaebacteria are monolayer (in stead of bilayer) of tetraether lipids in which both tails of hydrocarbon chains of two diether lipids are covalently connected in a tail-to-tail fashion. Although the host cell from which contemporary eukaryotes have been derived by endosymbiosis, is speculated to be an archaebacterium, the unique ether lipids raised a serious question to the idea of archabacterial origin of eukaryote cells; why the unique ether lipids are not used to construct cytoplasmic membranes of eukaryotes?

The author and his colleagues have studied biosynthesis of membrane lipids of two thermo-acidophilic archaebacteria, Thermoplasma and Sulfolobus. It was found that origin of stereospecificity of glycerol moiety of archaebacterial ether lipids differs from species to species. In Sulfolobus sn-glycerol-1-phosphate (the abnormal isomer of glycerol phosphate) seems to be directly synthesized from glycerol, whereas in Halobacterium stereospecificity of glycerol phosphate is inverted during the lipid synthesis.

Recently we found that specific inhibitors for eukaryotes squalene epoxidase inhibit the condensation of diether lipids to tetraether lipids in cell-free extracts of these thermophilic archaebacteria. The results suggest evolutionary implication of archaebacterial tetraether condensing enzyme to eukaryote sterol biosynthesis. Relationships between chemical structures of membrane lipids and early evolution of life will be discussed.

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ORIGIN OF FATTY ACIDS

The appearance of fatty acids and membranes is one of the most important events of the prebiotic world because genesis of life required the compartmentalization of molecules. Membranes allowed cells to become enriched with molecules relevant for their evolution and gave rise to gradients convertible into energy. By virtue of their hydrophobic/ hydrophilic interface, membranes developed certain enzymatic activities impossible in the aqueous phase. A prebiotic cell is an energy unit but it is also an information unit. It has a past, a present and a future.

The biochemistry of fatty acids involves acetylCoA, malonylCoA and an enzyme, acyl synthetase, which joins both molecules. After substitution of the acetyl group in place of the carboxyl group of malonyl derivatives, the chain is reduced and dehydrated to crotonyl derivatives. These molecules can again react with malonylCoA to form an unsaturated chain; they can also undergo a new reduction step to form butyryl derivatives which can react with malonylCoA to form a longer aliphatic chain. The formation of malonylCoA consumes ATP. The reduction step needs NADPH and proton. Dehydration requires structural information because the reduction product is chiral (D configuration). It is unlikely that these steps were possible in a prebiotic environment. Thus we have to understand how fatty acids could appear in the prebiotic era.

This hypothesis about the origin of fatty acids is based on the chemistry of sulfonium ylides and sulfonium salts. The most well-know among these molecules are S-methyl-methionine and S-adenosyl methionine. The simplest sulfonium cation is the trimethylsulfonium cation. Chemists have evidence that these products can produce olefin when they are heated or flashed with UV light in some conditions. I suggest that these volatile products can allow the formation of fatty acids chains in atmospheric phase with UV and temperature using methanol as starting material. Different synthetic pathways will be studied.

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ORIGIN OF NUCLEIC ACIDS

The appearance of nucleic acids is the first event after the birth of membranes which made it possible to assure the perenniality of information. The complexity of these molecules has led some scientists to propose that they were not prebiotic ut rather derived a more simple and achiral primitive ancestor. This hypothesis suggests that ribose possesses properties that allowed the formation of certain polysaccharides which evolved to RNA.

The first step of the hypothesis is the selection and concentration of ribofuranose. This sugar has chelating properties and its alpha-ribofuranose is favoured in the chelating position. The density of the sugar with a heavy cation is greater than water and thus the complex can escape the UV radiation at the surface of the ocean. The particularity of ribose is to be able to form a homochiral regular array of these basic chelating structures with pyrophosphite. These arrays evolve towards the formation of polysaccharides (poly ribose phosphate) which have a very organized structure. These polysaccharides in turn evolve to RNA by binding of adenine and deoxyguanine which are HCN derivatives that can react with the polysaccharides. The primitive RNA is methylated and oxidized to form prebiotic RNA with adenosine, cytidine, 7methyl-guanosine and ribothymidine as nucleic bases.

The pathway of biosynthesis of DNA from RNA will be studied.

I suggest that the appearance of DNA results from the interaction between prebiotic double stranded RNA and proteins. DNA could be a product of RNA degradation by proteins. The catabolism of RNA to DNA requires a source of free radicals, protons and hydrides. RNA cannot produce free radicals, which are provided by the phenol group of the amino acid tyrosine. Protons are provided by the medium and hydrides are provided by 7-methyl-guanosine which can fix hydrides coming from hydrogen gas and donate them for the transformation of a riboside to a deoxyriboside. This pathway suggests that DNA appeared at the same time as RNA. Like oxygen gas, DNA was a useful waste.

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In situ exploration of Titan and cometary nucleus : implication for Planetary Exobiology

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Initially limited to the search for extraterrestrial life, the field of exobiology progressively became the study of the origins, distribution and evolution of life in the universe. Its approaches are numerous and largely diversified. They include the study of the origins of life on Earth, the search for life, of its clues or traces outside the Earth, but also the search for extraterrestrial molecules and chemical processes related to life.

Although rare, there are places in the solar system concerned with the direct search for extraterrestrial life : Europa, one of the satellite of Jupiter, and, first of all, Mars. There are also numerous other places in the solar system interesting exobiology, not for a direct search for extraterrestrial life, but for studying organic chemical processes which are involved in their environment. The most important are comets and Titan : two very ambitious missions with planetary probe or lander are already programmed and prepared for the Horizon 2000 to explore those planetary bodies.

The Cassini-Huygens mission includes a US (NASA) spacecraft (named Cassini) which will carry a European (ESA) probe (named Huygens). It will be launched in October 1997 to reach the Saturnian system in 2004. There, the spacecraft will become artificial satellite of Saturn and of its biggest (natural) satellite Titan, and it will send the Huygens probe in its dense and organics-rich atmosphere. After entering the atmosphere, the probe will slowly descent with a parachute down to the surface. During the 2.5 hours of descent, six instruments will perform physical (wind, photon fluxes, electrical conductivity, T, P, ..) and chemical (nature and abundance of the organic and inorganic compounds present in the atmosphere, in gas and condense phases). These instruments include T, P, electrons sensors, MS, GC-MS and Pyr-GC-MS techniques. This will be the second GC-MS instrument never flown in a planetary mission (after Viking). The probe will also be able to perform surface measurements, with these instruments (the GC-MS should survive after impact), as well as with a dedicated Surface Science Package. SSP includes many sensors to measure and analyse Titan's surface (refractometer, densitometer, conductivity measurement etc).

The second (in chronological order) most ambitious planetary mission of the 21rst century is the "Rosetta" mission. It is a cometary mission, decided by ESA. It includes a spacecraft (named Rosetta) which will carry two landers : a French-US (named "Champollion") and a German (named "Roland", as Rosetta Lander). Rosetta will be launched in 2003. It will reach a comet in .... 2011 and then it will follow it closely for several years. It will also release Champollion and Rosetta which will land on the nucleus of the comet and perform many in situ measurements. Crucial scientific returns of exobiological importance are expected from instruments dedicated to the detailed study of complex organics likely to be present. in the cometary nucleus Among the possible instruments to be selected are a Pyr-GC-MS and an instrument measuring optical activity. The announcement of opportunity asking the scientific community for proposing instruments onboard the Rosetta spacecraft and its two landers has been released on March 1rst 1995. The selection process of instrument proposals on both landers has just started and the proposers are now impatiently waiting for its results.

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"La Grande Galerie de l'Evolution" of Paris: The only Museum in the world entirely devoted to biological evolution.

The new building called "Grande Galerie de l'Evolution" of the national Museum of natural History, in Paris-France, is the first museum in the world exclusively devoted to biological evolution.

Inaugured in june 1994, this building was the result of a huge national project of renovation concerning few large french science museums. From a scientific popularization point of view, showing to public, in a museum, the processes and results of biological evolution was a sort of challenge. Our choice fell on few major topics: diversity of life, consequences of interaction between man and nature, and the main processes of biological evolution along the story of life. These topics are developed with the help of the presentation of many animal (or plant) specimens belonging to the Museum collections.

The Museum is divided in 3 parts (named "Acts") :

- The aim of Act 1 is to sensibilize the visitor to the results of 4 billions years of biological evolution. This act shows some examples of biological diversity through few terrestrial and marine environments (deserts, tropical forests, polar habitats, abyssal zones ...).

- Act 2 is the principal part of the Museum explaining the main processes of evolution. This part shows also the story of life from the first living cells to man.

- Act 3, the last part offers to visitors a vision of the interactions between man and nature, and of their consequences along millions of years.

A special Gallery is :entirely devoted to vanished and threatened species, as a nefast consequence of human interaction on biological diversity particularly since the beginning of this century.

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`New Approaches in Mathematical Biology:Information Theory and Molecular Machines"

ABSTRACT

My research uses classical information theory to study genetic systems. Information theory was founded by Claude Shannon in the 1940's and has had an enormous impact on communications engineering and computer sciences. Shannon found a way to measure information. This measure can be used to precisely characterize the sequence conservation at nucleic-acid binding sites. The resulting methods, by completely replacing the use of ``consensus sequences", provide better models for molecular biologists. An excess of conservation led us to do experimental work on bacteriophage T7 promoters and the F plasmid IncD repeats. The wonderful fidelity of telephone communications and compact disk (CD) music can be traced directly to Shannon's channel capacity theorem. When rederived for molecular biology, this theorem explains the surprising precision of many molecular events. Through connections with the Second Law of Thermodynamics and Maxwell's Demon, this approach also has implications for the development of technology at the molecular level. Discussions of these topics are held on the internet news group bionet.info-theo.

INFORMATION-PROCESSING GENES

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ABSTRACT

DNA computing is an active interdisciplinary area of research. Our theoretical work and a recent laboratory experiment by Adleman clearly demonstrate that nucleotide sequences are capable of solving NP-complete (or computationally intractable) problems. We reached this conclusion through an analysis of molecular fossils.

There are an estimated 100,000 genes in the human genome of which 97% is non-coding. On the other hand, bacteria have little or no non-coding DNA. Non-coding region includes introns, ALU sequences, satellite DNA, and other segments not expressed as proteins. Why it exists? Why nature has kept non-coding during the long evolutionary period if they it no role in the development of complex life forms? Does complexity of a species somehow correlated to the existence of apparently useless sequences? What kind of capability is encoded within such nucleotide sequences that is a necessary, but not a sufficient condition for the evolution of complex life forms, keeping in mind the C-value paradox and the omnipresence of non-coding segments in higher eukaryotes and also in many archea and prokaryotes.

The physico-chemical description of biological processes is hardware oriented and does not highlight algorithmic or information processing aspect. Any information-processing system has two independent components: the algorithm and its hardware implementation. However, an algorithm without its hardware implementation is useless as much as hardware without its capability to run an algorithm. The nature and type of computation an information-processing hardware can perform depends only on its algorithm and the architecture that reflects the algorithm. Given that enormously difficult tasks such as high fidelity replication, transcription, editing and regulation are all achieved within a long

linear sequence, it is natural to think that some parts of a genome are involved in these tasks. If some complex algorithms are encoded within these parts, then it is natural to think that non-coding regions contain processing-information algorithms.

A comparison between well-known automatic sequences and sequences constructed out of motifs in found in all species proves the point: noncoding regions are a sort of "hardwired" programs, i.e., they are linear representations of information-processing machines. Thus in our model, a noncoding region, e.g., an intron contains a program (or equivalently, it is an automaton) while an exon contains acceptable data in the language of this automaton.

There are many important questions that we shall discuss in a monograph in preparation. These are:

Critical segments and their computational significance;
Long-range correlation in introns and their possible relevance to fractal nature of biological systems;
Anti-sense strategy and enzyme-directed therapy;
Evolution in the RNA world and molecular fossils;
Evolution of cellular communication system; and
The C-value paradox.

Susceptibility Discontinuity and specific heat anomaly in single crystal of alanine and valine

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ABSTRACT

Magnetization of single crystals of D-, L- Alanine and D-,L-, D,L-Valine were measured as functions of temperature. Susceptibility discontinuities were observed at 265 K for alanine and 270 K for valine by using Quantum Design SQUID magnetometer MPMS-5. The specific heat anomaly in D-, L-alanine and D-,L-, D,L-Valine measured by differential scanning calorimetry was shown that an obvious lambda transition at 270 K for alanine and 272 K for valine. The X ray powder diffraction analysis made on Liguka D/MAX-A using monochromat high intensity Cu-K showed that no crystal lattice changed but find a small peak produced under the temperature cooling down from 293 K, 273 K, 263 k and 123 K. We propose that the discontinuity is attributed to the change in the intramolecular electron spin at the orientational order-disorder transition. It was coincidence with the shape of the specific heat jump of electron coupling.

Amino Acid chirality Breaking by N-Phosphorylation

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The chirality breaking of amino acid is a focus issue in the origin of life. For chemists, there are some interesting chemical approaches to solve the symmetry breaking problem[1,2]. Our previous experiments indicated that when amino acids were phosphorylated, there were many bio-mimic reactions happened[3]. In this paper, it was found that there had significant difference between the N-phosphoryl L- and D- amino acids such as serine and threonine. The optical rotation tracing experiments of the racemic N-phosphoamino acids also showed the similar results. The chirality breaking of amino acids by N-phosphorylation was an novel phenomena.

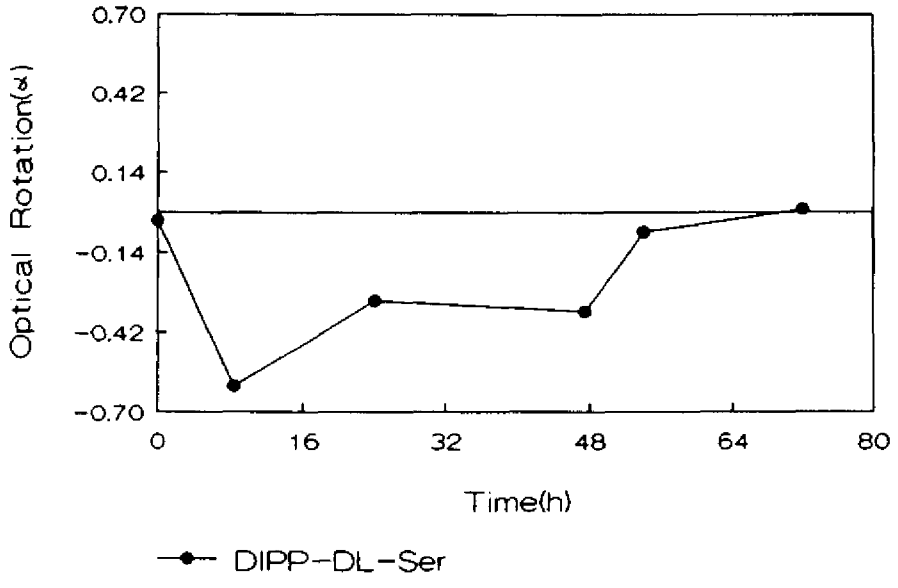

Figure 1

References:

1. C. Ponnamperuma, et al., J. Mol. Evol. 1980, 16, 153.

2. T.Tukuhara and S.Tuasa, ibid, 1991, 32, 304.

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