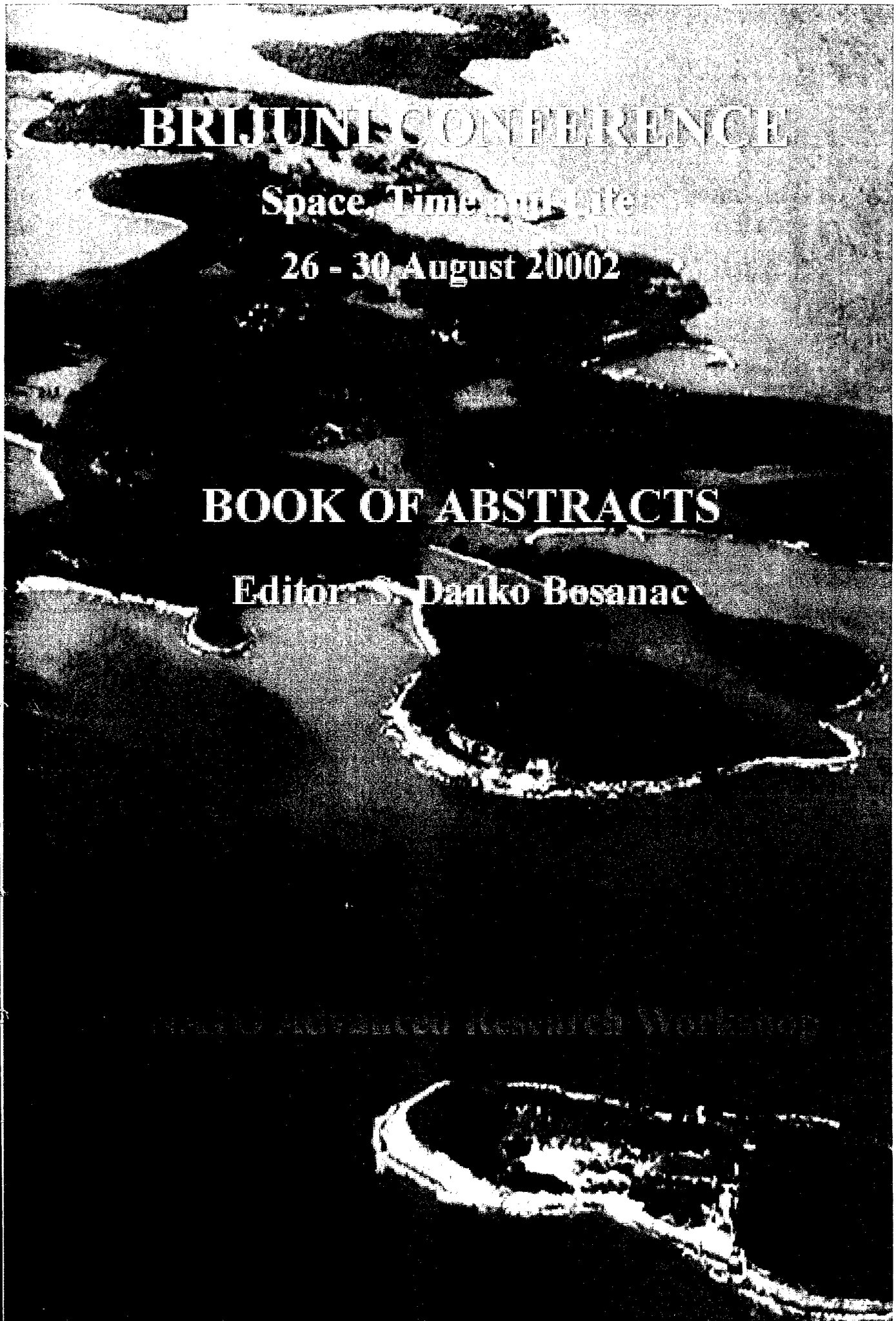

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PICNIC

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2. Abstracts

THE EMERGENCE OF LIFE; GEOCHEMICAL, MOLECULAR-BIOLOGICAL AND INFORMATIONAL CONSTRAINTS ON THEORY AND EXPERIMENT.

Gustaf Arrhenius
Scripps Institution of Oceanography,University of California, San Diego,La Jolla, CA 92093-0236

The questions concerning the origin and early evolution of life are mostly approached with focus on the complex problems of biomolecular autosynthesis. The specialists in this field are chemists and molecular biologists. They are seriously concerned with the staggering difficulties met in their own realm and tend to avoid dealing with the additional severe environmental limitations that are suggested by our general knowledge of planetary and spatial physics and chemistry. This purposeful neglect is often rationalized by the impression that their counterparts in the environmental sciences are groping in the dark and that, allowing enough time, shifting geochemical consensus will give back unlimited freedom to organic suppositions.

Planetary chemists on the other hand draw on their experience in studying present-day natural processes with reflection in the geological record. This makes them fit to attempt reconstruction of the environmental processes that may have controlled biopoesis. However, they often labor under the impression that any kind of organic molecule that can be conjured up in a harsh Archaean environment signifies the emergence of life.

The gap between the two cultures has been narrowed, but not closed, by the extensive interdisciplinary activities in this field, fostered chiefly by NASA and other national and international agencies with an interest in exploring the origin of life and the possibility of its emergence also on other worlds. The present meeting gives an opportunity for another step toward defining the central problems and for reviewing relevant progress. This presentation will aim at the following central topics:

" Environmental requirements for the generation of source molecules needed for metabolism and for generation and transduction of information
" Factors in the primordial planetary and spatial environments that favor constructive processes vs. detrimental conditions
" Physically and chemically realistic conjectures that can be made to overcome apparent hindrances
" Autosynthetic generation, encoding and propagation of molecules capable of information transduction
" Modeling of primordial metabolism
" Concentration and encapsulation of source molecules from highly dilute state; the improbability of a "primordial soup"
" Earliest planetary evidence for life and its relation to the phylogenetic tree on Earth

Brijuni Conference VIII, Brijuni, Croatia, 26.8.-31.8.2002.

DETERMINATION OF THE ATOM NUMBER DENSITY IN RUBIDIUM VAPOUR

D. Aumiler, T. Ban, R. Beuc and G. Pichler
Institute of Physics, Bijenička 46, P.O. Box 304, HR-10001 Zagreb, Croatia

A new method for the atom number density determination in alkali vapour is proposed. The method is based on the comparison of numerical simulation of the alkali self-broadened resonance lines absorption profiles with measured ones. The numerical simulation calculates absorption profiles starting from the relevant set of alkali *ab initio* potential curves, using semiclassical stationary point approximation. As a result, the reduced absorption coefficient (absorption coefficient divided by the square of the atom number density) is obtained. By adjusting the temperature parameter of the model, it is shown that in the spectral region around resonance lines excellent agreement between simulated and experimental absorption profiles can be achieved. The least squares fitting of the simulated profiles to the measured profiles determines the vapour temperature with the uncertainty of less than ±1°C. The measurements were made on rubidium vapour generated in a homemade crossed heat-pipe oven. In this way we were able to measure the Rb atom number densities with accuracy better than ±3%.

The advantage of this method is that the measurement of the sole physical quantity – absorption coefficient is sufficient for the accurate determination of the atom number density. In particular, one does not need to know the temperature of the vapour in order to determine the atom number density. This is especially important in experiments in which exact vapour temperature measurements are not possible, as is the case when a heat-pipe oven is used. Similar application of the method could also be found in plasma diagnostics of pulsed high-pressure alkali light sources, which we are currently investigating in our laboratory.

APPLICATIONS OF ARTIFICIAL NEURAL NETWORKS FOR MODELLING CONTROLLED RELEASE SYSTEMS.

Jadson C. Belchior*
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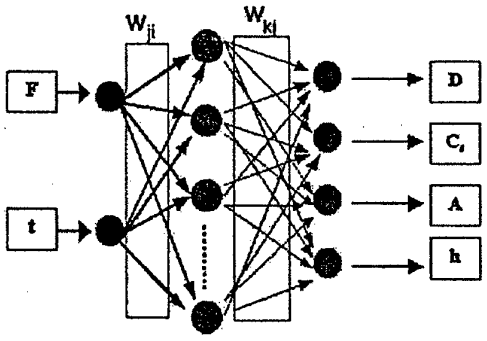
Pampulha, (31.270-901) Belo Horizonte, MC – Brazil

Efficient controlled release systems are fundamental for efficient therapeutical methodologies mainly to improve drug treatment through rate and time programmed drug delivery. However, the occurrence of multicomponents instead of single drug diffusion may complicate the ex- perimental procedure to produce adequate drug delivery systems. Therefore, mathematical models of controlled delivery systems are important to simulate the device properties such as the geometries and physicochemical properties of the system.



This work presents an alternative methodology, based on artificial neural networks (see figure) to study drug delivery systems. A drug model system of hydrocortisone was selected to test the present approach but introducing modifications to increase complexity. The results of the neural network obtained after the learning stage can be considered quantitative to predict an ideal experimental condition. The analysis of the outcome results has shown that one can predict properties of an efficient experiment with a relative average error smaller than 2%.

Figure: Artificial neural network. Input layer (F - drug fraction released and t - time), an intermediary layer and an output layer (diffusion coefficient (D), saturation solubility (C,), initial drug load (A) and height of the device (h)).

*Work supported by CAPES, FAPEMIG and CNPQ, Brazil.

SEMICLASSICAL APPROACH TO THE DESCRIPTION OF COLLISIONALLY INDUCED OPTICAL TRANSITIONS OF DIATOMS

R. M. Beuc and M. Movre
Institute of Physics, Institute of Physics, Bijenička 46, P.O. Box 304
HR-10001 Zagreb, Croatia

In a recent paper by Devdariani et al. [1], a formula was obtained that describes asymptotically forbidden quasimolecular optical transitions in the frame of the semiclassical approach. The main difficulty in the analytical description of asymptotically forbidden transitions is the consequence of the simple fact that the transition moments in this situation cannot be approximated by constant values as in the case of allowed transitions. However, potential energy curves and optical transition probability (or radiation width) usually can be reasonably approximated by exponential functions and a general formula which covers the central part of the spectral line, the extremum vicinity and the far wings, and also takes into account the fast exponential change in the state radiative width, can be obtained with the use of the Morse potential for the potential energy difference.

Our approach is based on a refinement of the theoretical model, based on the uniform Airy approximation as presented by Beuc and Horvatic [2]. The main point is careful treatment of the phases corresponding to the relevant Condon points and the resulting interference effects which in the same time take care of the variable transition moment in the vicinity of an extremum in the curve describing the difference between the electronic energies of the initial and the final states of the optical transition.

Bieniek et al. [3] have analyzed analogous processes of ionizing collisions in complex potentials within uniform JWKB stationary-phase techniques. Their numerical results are in excellent agreement with fully quantal, complex-potential computations. Our new results additionally support conclusions reached in [2] and [3] that the unified Franck-Condon theory is capable to describe asymptotically forbidden but collisionally induced transitions.

[1] A. Devdariani, E. Bichoutskaia, E. Tchesnokov, T. Bichoutskaia, D. S. F. Crothers, E. Leboucher-Dalimier, P. Sauvan and P. Angelo, J. Phys. B.: At. Mol Opt. Phys. **35** (2002) 2469-2475

[2] R. Beuc and V. Horvatic, J. Phys. B: At. Mol. Opt. Phys. **25** (1992) 1497-1510

[3] R. J. Bieniek, M. W. Müller and M. Movre, J. Phys. B: At. Mol. Opt. Phys. **23** (1990) 4521-4538

Brijuni Conference VIII, Brijuni, Croatia, 26.8.-31.8.2002.

THE EARLIEST STAGES OF STAR FORMATION

Leo Blitz
University of California at Berkeley, Radio Astronomy Laboratory, 635 Campbell 3411, Berkeley, CA-94720-3411, USA

Serious searches for signals from technological civilizations will be greatly enhanced by a new generation of radio telescopes, the first of which is currently under construction by the Radio Astronomy Laboratory at Berkeley. The probability that the searches will be successful depends, among many other things, on how commonly the conditions conducive to the development of life are found in the Milky Way. The birth of stars and planetary systems takes place in giant clouds of molecular gas and dust which are remarkably similar to one another throughout the Milky Way and in nearby galaxies. The sun-like stars that form within them inevitably have protoplanetary disks that have a large range in properties and are affected by environmental differences. If biological evolution requires catastrophic events such as bombardment by cosmic debris, the evidence suggests that although planetary systems vary greatly, such debris is common. Its distribution, and thus the likelihood of colliding with an earth-like planet, depends on the details of planet formation. Although the formation of earth-like sytems is probably not as common as previously thought, recent evidence suggests that the differences bewteen systems are less important than their similarities.

LASER CONTROL: ANALITICAL SOLUTION OF THE THREE LEVEL SYSTEM DYNAMICS

D. Bonacci, S.D. Bosanac, N. Došlić
'Ruđer Bošković' Institute, Bijenička 54, 10000 Zagreb

Many systems of current interest in physical chemistry are too complex for the full analitical treatment. For example, laser control parameters for manipulation of molecular state population are generaly optimized numericaly. Although the advancement of computer technology eliminated the time consuming note from this approach, it still lacks the depth of theoretical insight that even aproximate analytical calcultion would yield.

We obtained analitical solution of the specific three-level system in strong coherent electric field, extending in this way the classical Rabi theory developed half a century ago for two-level systems. Analitical solution enabled us to explore some details of the system's dynamics, and to determine the relative importance of various physical parameters of the system.

THE FUTURE OF LIFE

Charles R. Cantor, PhD
SEQUENOM, Inc., San Diego, CA USA

All living organisms have properties that are a convolution of their genetic programming and environmental exposure. Until recently humankind has had only a feeble ability to modify the genetic programming of organisms, but in recent years this has changed dramatically. We now can pretty much do anything we want. However, our current ability to predict the outcome of genetic manipulations is still extremely limited. In parallel, humans have also gained the ability to manipulate the environment. While we are far away from total control, globally, we can do pretty well, locally.

The result of these advances in technology is that future evolution of all life on our planet will be pretty much controlled by humans. We will see the emergence of newly designed species with enhanced properties to communicate, regenerate, produce energy efficiently, generate fuels, synthesize medicines, and manufacture healthier (for humans) food. We will also witness the directed evolution of humans with enhanced properties. Clearly this will not occur without some controversy.

It is probably a natural outcome of evolution that a species attains the ability to control and accelerate its own evolution. However, this great power to improve also comes with an equal power to do harm, and no single technology has greater power to threaten our stability as a society than biotechnology, if used malevolently.

BRIDGING FROM MICRO TO MACRO BY MEANS OF MESOSCOPIC SIMULATIONS IN PHYSICS AND BIOLOGY

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ITALY

An impressive range of results has been obtained in the field of Molecular Dynamics in the last decade for systems up to the size of about 100 nm. Due to the enormous potential for technological applications at the macroscopic level it is necessary to go well beyond such a limit. However, the computational costs of increasing the size of the system of even one or two orders of magnitude are absolutely proibitive. A suitable alternative may be to split up the problem according to the different length scales involved, i.e. Multiscale Modelling (MM). Several approaches have been proposed for MM: in general they start from atomistic simulations, replacing, however, the interatomic interactions with e.g. interactions among dislocations or, for larger systems, among dislocation densities or grains. However, since our major concern lies in the macroscopic domain (e.g. NDE or materials characterization), we propose to reverse this "bottom-up" strategy.

The approach we propose starts with a very fine discretization of the macroscopic specimen under study, which brings us to the mesoscopic level. For this bridging from a microscopic to a macroscopic scale by means of mesoscopic simulations, we plan to use the local Interaction Simulation Approach (LISA), whose "local" nature makes it ideally suitable for the task in hand, particularly in the case of strong local heterogeneities. Due to the complexity and vastness of scope of our goal, rather than searching for a general recipe, we propose to investigate several "case studies", which should demonstrate the feasibility of the approach and its validity. A similar approach can be used in biology and medicine to bridge between cell dynamics and macroscopic problems, such as the simulation of growth and therapy of tumors.

PROTON TRANSFER IN ACETYLACETONE: AN AB-INITIO STUDY

G. Kovačević , I Matanović and N. Došlić
R. Bošković Institute, Bijenička 54, Zagreb Croatia

Reaction minima and transition states, concerning proton transfer in acetylacetone were determined using M\o ller-Plesset ab initio and B1LYP density functional theory calculations. It is found that the minima and the transition state for proton transfer have different methyl groups orientation. Intrinsic reaction path calculation has shown that the rotation of the methyl groups is not concerted with the proton transfer reaction, rather they are consecutive processes. The thermodynamical stability of the keto and enol forms of acetylacetone is explored by using G2 type calculations and it is shown to be in good agreement with experimantal results.

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THE TIME VARIABLE IN THE NEURAL ENCODING OF CONSCIOUSNESS STATES

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That *time* plays an important role in the so-called NCC (Neural Correlate of Consciousness) has been suspected for long time, both because *synchrony* appeared to be critical for the binding of the various features building a conscious representation, and from the experimental observation of stronger *oscillations* of the electric field associated with the performance of a cognitive task when performed in a conscious way.

Nevertheless, although probably 'in the air' for more than a decade, the simple theory claiming that consciousness is characterized by the encoding of its content into a *purely temporal pattern*, irrespectively of the identity of the neurons involved, has been either ignored or rejected, although having been the subject of 3 recent works (Helekar 1999, Durup and Sanejouand 2000, John 2001).

We shall show that the combination of largely accepted experimental data with insights from evolution theory allows us to give a *demonstration* of the above-stated theory, on the basis of the immense ratio between the capacities of non-conscious *vs* conscious processing.

Important differences between the models which have been developed within this theory will be discussed: (i) is the code universal or individual ? (ii) are the relevant neural computations performed with bits or with qubits ?

Finally, and in an unrelated way, we will show that a well-known aspect of consciousness, namely its limited content, allows us to give an elegant answer to the old philosophical problem: free will or determinism ?

CONTROLLING OPTICAL DIFFRACTION AND DIRECTIONALITY FROM A SUBWAVELENGTH APERTURE

Thomas W. Ebbesen
ISIS, Louis Pasteur University, 4 rue B. Pascal, 67000 Strasbourg, France

Materials structured on the nanometer scale can lead to improved and sometimes surprising properties. This will be illustrated in some detail by our own work on the extraordinary optical properties acquired by metal films when their surfaces are corrugated and perforated with one or more sub-wavelength holes (~150 nm). Such structures can transmit the light with an efficiency hundred times larger than what theory predicts for single holes. The efficiency can even be much larger than the fractional area occupied by the hole, which means that even the light falling beside the hole emerges on the other side of the sample. This extraordinary transmission is due to the coupling of the incident light with the surface plasmons of the film. The transmission spectrum contains peaks attributed to surface-plasmon modes that depend on both the symmetry and the 2D lattice parameter of the surface corrugation. Novel results show that an other fundamental problem of sub-wavelength apertures, namely optical diffraction, can also be modified using surface plasmons. The optical divergence and directionality of light transmitted by a single subwavelength aperture can be controlled. These results have broad fundamental and practical implications and show that, with modern fabrication techniques, surface plasmons can be engineered to yield unique optical properties.

Ref.: Ebbesen et al Nature 391, 667 (1998); Ghaemi et al, Phys. Rev. B 58, 6779 (1998); Grupp et al Adv. Mater. 11, 860 (1999); Kim et al, Optics Letters 24, 256 (1999); Grupp et al, Appl. Phys. Lett., 77, 1569 (2000); Martin-Moreno et al, Phys. Rev. Let.. 86, 1114 (2001); Krishnan et al. Optics Comm. 200, 1 (2001); Lezec et al Science, in press (2002).

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BIOLOGICAL INFORMATION AND PHASE TRANSITIONS

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MPI fuer Biophysikalische Chemie, Goettingen

Information has two aspects: a quantity to be called "extent" and a quality which may be termed "content" since it deals with meaning. The latter originates via selective self-organization which can be described also in quantitative physical terms. A prerequisite is the reproducibility of the informational substrate forming the basis of selection. This paper focuses on selection being the analogue of a physical phase transition. In the first part the criteria for phase transitions are formulated. The second part introduces the concept of information space and describes information as selected points or regions in this space. In the third part selection is analysed in terms of the criteria for phase transitions, and finally the concept is confronted with experimental data. The conclusion is reached that information content is generated via selection which can be described as a phase transition in information space.

ORIGIN AND PERSISTENCE OF GENETIC MATERIAL IN PREBIOTIC HABITATS

Enzo Gallori
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Molecules which store genetic information (RNA, DNA) are central to all life on earth. The formation of these complex molecules required specific conditions, including the synthesis of precursors (nucleotides), the joining of these monomers into larger molecules (polynucleotides), their protection from degradation, and the expression of the biological potential of the informative molecule, which is its capacity to multiply and evolve. Determining how these steps occurred and how the earliest genetic molecules originated on Earth is a problem that is far from being resolved. Classical research in this field has focused on process in aqueous solution. However, it is difficult to believe that complex molecules can be obtained by random collisions in a fully aqueous environment since under these conditions, hydrolysis and not polymerization if favoured.

We believed that it is crucial to consider surface organic chemistry.

As early as 1951, J.D. Bernal suggest, on the basis of thermodynamic and kinetic considerations, that mineral surfaces (specifically clay minerals) could have played an important role in the prebiotic formation of the biomolecules basic to life.

In recent years, numerous observations in different fields, from astrophysical chemistry to molecular biology, have reinforced the hypothesis of the involvement of mineral surfaces in the prebiotic origin of life.

OVERVIEW OF THE CONFERENCE

Martin Harwit
Cornell University, Department of Astronomy, Ithaca, NY 14853-6801, USA

This conference covers the entire range of issues --- cosmological, astronomical, geophysical, chemical, biological, and neurological --- dealing with the questions "How did we get here? How is it that we are even able to ask this question?" This final talk will attempt to summarize what the previous speakers have taught us and to assemble their thoughts into a coherent thread.

MOLECULAR DYNAMICS SIMULATIONS OF THE INFRARED SPECTRUM OF BENZALDEHYDE

T. Hrenar(1), R. Mitrić(2) and Z. Meić(1)
(1) Faculty of Science, University of Zagreb, Strossmayerov trg 14, HR-10000 Zagreb, Croatia
(2) Humboldt Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2 12489 Berlin

A calculation of vibrational spectra with semiempirical or ab initio force fields gives generally too high values for vibrational frequencies. However, the use of the density functional methods (DFT) reduces the need for correction of frequencies or the corresponding force constants. On the other hand, calculations of vibrational spectra by molecular dynamics methods do not demand such empirical corrections.

With the calculated ab initio force fields we have carried out Newtonian dynamics. From the time dependency of the dipole moment one can deduce information on infrared (IR) spectra of molecules. The described method is applied to benzaldehyde, which is a proper molecule due to its size and availability of experimental data. The obtained results will be presented and discussed.

ARE EARTH-LIKE PLANETS GOING TO BE DISCOVERED SOON?

Michael Jura
Department of Physics and Astronomy, University of California, Box 951547, Los Angeles, CA 90095-1547, USA

Jovian-mass planets and ``pebbles" as large as 5 cm in diameter have been inferred to orbit nearby stars. However, to date,there has been no direct evidence for the existence of terrestrial-mass planets, although we strongly suspect that such planets exist.

In this talk, the evidence for the existence of extra solar-system asteroids will be reviewed, and strategies for the discovery of terrestrial mass planets will be discussed. Methods to search for life on these hypothetical planets are part of this program.

LIFE AND ENTROPY PRODUCTION

Davor Juretić
Department of Physics, University of Split, Nikole Tesle 12, Split, Croatia

Nobody disputes that life creates entropy, but whether living systems augment or diminish the rate of entropy production is still an unresolved question. Do living entities make the least concession possible to entropy by seeking the steady state of minimal entropy production, or do they maximize the rates of dissipation?

We shall use several simple models for cyclic biochemical reactions to calculate entropy production and efficiency of free-energy conversion in a steady state. Our goal will be to explore whether actual operation of these cycles can be better modeled by requiring minimal or maximal entropy production. An optimization principle coming from physics would surely help in predicting behavior of complex metabolic networks revealed after the completion of different genome projects.

Main attention will be devoted to bioenergetics of bacterial and plant photosynthesis, and to ATP driven biochemical cycles.

3+1 IS MORE THAN ENOUGH – PARTICLES IN LOWER DIMENSIONS

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The topological approach is developed where an elementary particle is considered as corresponding to a localised space-time configuration [1]. The key of the approach is the standard relativistic limit for space-time curvature. In general case, the space-time configurations, for which this limit is maintained, are shown to be three-, two-, and one-dimensional as space objects. The real space-time is proposed to consider as evolution of a mixture of one-, two-, and three-dimensional micro-objects, which interacts and compose macroobjects corresponding to its degrees of freedom in space co-ordinates.

In the frames of the approach presented, a photon is described as 2+1 configuration where abovementioned condition is valid in its centre point. The configuration possesses of Doppler effect behaviour in the case it propagates with light velocity only. Topological charge of the configuration is zero. The photon spin is represented as configuration' rotation around the propagation direction; the only permissible rotation period corresponding to the photon wavelength. It is shown that ordered one-dimensional superposition of single-photon configurations composes a restricted stable coherent harmonic-type packet which wavelength equals to the constitutive photon configurations' wavelength. Two- and three-dimensional coherent superpositions of single-photon configurations are shown to form some types of photons ordering symmetry inside the coherent packet.

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INTERMOLECULAR FORCES

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The characterization, at high spectral resolution, of molecular complexes has led to detailed knowledge of intermolecular forces. The structure and dynamics of stable and metastable states will be discussed. Of particular interest will be hydrogen bonded species as well as the rich variety of isomeric forms presently observed. We examine the question of whether and when weak interactions can modify dynamical pathways. Finally we discuss the structure of complexes of molecules with hydrogen and helium.

PANSPERMIA: MYTH OR REALITY?

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Panspermia, the hypothesis that life reached Earth from outer space, was developed by Svente Arrhenius between 1903 and 1906. This is the "strong" version of panspermia, and it sidesteps the question of how did life originate. There were several precursors who had suggested that life existed elsewhere in the Universe (Anaxagoras, Giordano Bruno, Fontanelle). There were also precursors such as Berzelius who, in 1834, suggested meteorites as carriers of life. But a scientific approach to these questions had to await the demise of the long-held concept of spontaneous generation and the development of Darwin's theory of evolution. As understanding of astronomical and astrophysical observations progressed, the concept of life elsewhere than on Earth had fluctuating fortunes, as did estimations of the probability of survival of space transit and atmospheric entry. Thus a more chemical/biochemical approach to the origin of life on Earth developed, one variant of which, involving the infall of prebiotic chemicals, constitutes a "weak" panspermia hypothesis. The scientific and, in part, philosophical background to these developments will be discussed and will include remarks on directed panspermia.

STEPS TOWARDS COMPLEX MATTER: INFORMATION, SELF-ORGANIZATION AND ADAPTATION IN MOLECULAR AND SUPRAMOLECULAR SYSTEMS

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One of the major lines of development of chemical science in the coming century resides in the ever clearer perception, deeper analysis and more deliberate application of information features in the elaboration and transformation of matter, thus tracing the path from merely condensed matter to more and more highly organized matter towards systems of increasing complexity.

A most basic and far-reaching contribution of supramolecular chemistry is the implementation in chemical science of the concept of molecular information and its corollaries, instructions and programmed chemical systems, with the aim of gaining progressive control over the organization of matter, over its spatial (structural) and temporal (dynamical) features.

Supramolecular chemistry is actively exploring systems undergoing *self-organization*, i.e. systems capable of spontaneously generating well-defined functional supramolecular architectures by self-assembly from their components. Self-organization processes may be directed via the *molecular information* stored in the covalent framework of the components and read out at the supramolecular level through specific interactional algorithms, thus behaving as *programmed chemical systems*.

The control provided by self-organization processes allows the development of *functional supramolecular devices*, defined as structurally organized and functionally integrated systems built from suitably designed molecular components performing a given function (e.g. photoactive, electroactive, ionoactive, etc.) and containing the features required for assembly into an organized supramolecular architecture. Self-organization processes also give access to advanced *functional supramolecular materials*, such as supramolecular polymers and liquid crystals.

The design of molecular information controlled, "*programmed*" self-organising systems provides an original approach to *nanoscience* and *nanotechnology*. In particular, the spontaneous but controlled generation of well-defined, functional supramolecular architectures of nanometric size through self-organization represents a means of performing programmed *engineering* and *processing* of *nanomaterials*.

Technologies resorting to self-organization processes are in principle able to provide a powerful alternative to nanofabrication and nanomanipulation procedures by making use of the spontaneous but controlled generation of the desired superstructures and devices from suitably instructed and functional building blocks.

Supramolecular chemistry is also intrinsically a *dynamic chemistry* in view of the lability of the interactions connecting the molecular components of a supramolecular entity. Furthermore, because of the ability of supramolecular species to exchange their constituents, they have also *combinatorial* capacity.

Consequently, supramolecular devices and materials are by nature *dynamic species*, whose constituents are linked through reversible connections and undergo spontaneous and continuous assembly/deassembly processes in a given set of conditions. Because of their intrinsic ability to exchange their constituents, they have also combinatorial character so that they may be considered as *dynamic combinatorial devices and materials*. Being instructed, dynamic and combinatorial, they may in principle select their constituents in response to external stimuli or environmental factors and therefore behave as *adaptive systems*.

The same considerations apply to molecular entities constructed from components linked through reversible covalent connections. Together, such molecular and supramolecular systems embody a *dynamic combinatorial chemistry*.

The merging of the features of supramolecular systems : - information and programmability, - dynamics and reversibility, - constitution and structural diversity, points towards the emergence of *adaptive chemistry*. A further development will concern the inclusion of the arrow of time, i.e. of non-equilibrium, irreversible processes and the exploration of the frontiers of chemical evolution towards the establishment of *evolutive chemistry*, where the features acquired by adaptation are conserved and transmitted. In combination with the corresponding fields of physics and biology, chemistry thus plays a major role in the progressive elaboration of a science of informed, organized, evolutive matter, a *science of complex matter*.

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"CASSCF/CASPT2 STUDY OF THE MECHANISM AND KINETICS OF THE GAS-PHASE OZONE ADDITIONS TO ETHENE, FLUOROETHENE AND CHLOROETHENE".

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"Ab initio multiconfigurational CASSCF and CASPT2 methods were employed in studying the reaction mechanisms and kinetics of the gas-phase ozone additions to ethene, fluoroethene and chloroethene. Reactants, transition state structures and products were optimized and harmonic vibrational frequencies calculated at the CASSCF/cc-pVTZ level. For kinetic calculations the electron energies of all the stationary points were further refined by utilizing the CASPT2 method with the optimized CASSCF/cc-pVTZ wavefunctions taken as the zeroth-order. The rate constants and Arrhenius kinetic parameters were finally calculated in terms of the conventional transition state theory. The favourable conformations of the ozone approach to the two asymmetrically substituted haloalkenes are at first governed by the electrostatic repulsion in the transition state structures and later by the gradually predominating anomeric effect. The bond formation in the primary haloozonides was analyzed by monitoring the changes in the occupation numbers of the active orbitals in course of the optimizations. For all the reactions thus studied a close agreement is found with the experimental kinetics, which makes a future use of the same approach very promising."

THE LIFE OF THE UNIVERSE

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Many results on the probability of life in the Universe assume that physics is close to a final answer, in particular that the theory of relativity is, at least, very approximately correct. But new astronomical observations and theoretical work suggest otherwise. Perhaps the Universe changes its laws as it expands, the constants of nature are wildly different near black holes and other high concentrations of matter, and ultimately the ``nothing can travel faster than light" dogma is not entirely correct. I examine these possibilities with reference to what they may imply to life in the Universe, and our prospects of ever establishing communication with alien civilizations.

MATTER, LIFE, AND INFORMATION PHASE TRANSITIONS OF THE UNIVERSE

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In classical physics, space, time, and matter were considered as basic concepts of a steady-state universe. In the framework of modern science, the universe is no longer a dead mechanical clockwork: It seems to evolve as a self-organizing complex system according to phase transitions with the emergence of new materials, life, consciousness, and intelligence. Life is no random event at the edge of the universe. Are we alone? What are the common structures and laws of this development? In the age of computers, computer simulations and computer experiments deliver first insights into the information processing of complex systems. Information itself seems to be a fundamental ingredient in the evolution of the universe. These concepts of modern science lead back to ancient ideas in the philosophy of nature.

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EXTRASOLAR PLANETARY SYSTEMS: FROM INDIVIDUAL DETECTIONS TO STATISTICAL PROPERTIES

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The discovery of planets around other stars was (up to now) only possible due to the development of high-precision radial-velocity techniques. These techniques have permitted astronomers to look for the tiny periodic motion of a star as it moves around the center-of-mass of the star-planet system. Radial velocity surveys have revealed up to now about 100 extra-solar planets and 9 multi-planetary systems. The discovered planets present a wide variety of orbital element and masses, which are raising many problems and questions regarding the processes involved in their formation. But the analysis of the distributions of orbital elements, like the period and eccentricity distributions is already giving some constraints on the formation of planetary systems. Furthemore, the study of planet host stars have revealed the impressive role of the stellar metallicity on the giant planet formation. The chemical composition of the molecular cloud is probably one of the key parameters to form giant planets. The study of extra-solar planetary systems is just giving its first steps. After only 7 years, we can say that at least 5% of the solar type stars have giant planetary companions with masses as low as the mass of Saturn and orbital periods less than about 5 years. But the understanding of how giant planets are formed is still shaded in many points and we are still lacking of any detections of analogs of terrestrial planets. To help solve some of these problems, several projects are currently in the pipeline. Future space missions, like the photometric missions COROT, Eddington or Kepler (to search for planetary transits) or the astrometric satellites GAIA and SIM will definitively permit to unveil hundreds (or even thousands) of "new" planets. But ground based astronomy will also give enormous steps in the next few years.

TIME OPERATOR IN QUANTUM MECHANICS

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Controversy about the existence of a self-adjoint time operator , T , conjugate to a given Hamiltonian is reexaminated. Specifically , we attempt to obtain an explicit solution to the operator equation -i [T (p,q) , H (p,q)] = 1 for a conformally invariant Hamiltonian. References: 1. V. de Alfaro, S. Fubini, G. Furlan: Nuovo Cimento 34A, 569 (1976). 2. C.M. Bender, G.V. Dunne: Phys.Rev. D40, 2739 (1989). 3. H.R. Lewis, W.E. Lawrence, J.D. Harris: Phys. Rev. Lett. 77, 5157 (1996).

NANOTUBES: NUMBER OF KEKULÉ STRUCTURES AND AROMATICITY

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Carbon nanotubes (CNTs) are composed of cylindrical graphite sheets consisting of sp^2 carbons. Due to their structure CNTs are considered to be aromatic systems. In this work the number of Kekulé structures (K) in CNTs was estimated by using the transfer matrix technique. All Kekulé structures of the cyclic variants of naphthalene and benzo[c]phenanthrene have been generated and the basic patterns have been obtained. From this information the elements of the transfer matrix were derived. The results obtained indicate that K (and the resonance energy) is greater if tubulenes are extended in vertical than in horizontal direction. Tubulenes are therefore more stable than cyclic strips.

A SPIN LABELLING STUDY OF THE HYDROPHOBIC BARRIER IN LIPOSOMES

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A fundamental property of biological membranes is to act as a barrier to permeation of polar molecules. This barrier effect is largely due to a hydrophobicity of a phospholipid bilayer, determined by the extent of water penetration into the membrane.

In order to study the depth of water peneration into liposomes, we used the electron spin echo modulation, a pulsed electron spin resonance method [1], that takes advantage of the solvent effect on the hyperfine interaction of the nitroxide spin labels. A fatty acid with the paramagnetic nitroxide group of the spin label covalently attached at various positions along the fatty acid chain was introduced into the multilamellar liposomes. The hydrophobic barrier for water molecules, as well as, for small molecules such as glycine, was studied as a function of the liposome composition and size.

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Brijuni Conference VIII, Brijuni, Croatia, 26.8.-31.8.2002.

ON THE COSMIC CONNECTION OF FUNDAMENTAL PARTICLES AND FIELDS

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We observe that, on the scene of Space and Time, the Matter arranges itself in ways that provide a chain of coincidences enabling creation of Life and intelligent creatures. While the broadest principles of Special Relativity and Quantum Mechanics provide merely a language, a further insight into the selection of particles and forces existing in the universe comes from the local Gauge Symmetries. The other cherished symmetries of the particle physics are awaited to be violated towards the more fundamental scale, probed in the early universe.

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MODELING OF BOILING POINTS OF BENZENOID HYDROCARBONS REVISITED

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Polycyclic aromatic hydrocarbons and their subset benzenoid hydrocarbons are a class of mutagenic and/or carcinogenic environmental pollutants being permanently formed by incomplete combustions. As benzenoids are ubiquitous pollutants new information about their properties and features as well as their biological activity are desirable and important.

The normal boiling point *per se* is an important feature of a compound, moreover it is one of the indispensable physicochemical properties for a reasonable risk assessment of a chemical. Hence, several QSPR (quantitative structure property relationship) studies of the normal boiling points of smaller benzenoid hydrocarbons have recently been carried out. Many of the normal boiling points used in the training set in all these studies differ considerably from the corresponding data in the sources like Beilstein, Merck Index, and others. For example, the normal boiling point of coronene in these studies is 590 ^{0}C, but according to the aforementioned reliable sources it is 525 ^{0}C!

We have carried out a novel QSPR study of the normal boiling points of benzenoid hydrocarbons using data from Beilstein and different topological indices as predictor variables. The developed models are mutually compared and some of them are of high quality.

``SIGNATURES OF MATTER-ANTIMATTER ASYMMETRY IN THE COSMIC MICROWAVE BACKGROUND RADIATION?''

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Helical primordial magnetic fields could be expected from cosmic events such as electroweak baryogenesis. Such fields can lead to helical velocity flows and could manifest themselves as non-vanishing correlations of the temperature and B-type polarization of the CMBR. Primordial helical magnetic field can also be detected using Faraday rotation measure maps of the CMBR.

SELF-ORGANIZATION FROM SPACE TO LIFE

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Self-organization laws determine all natural processes from Space to Life. It is known the role of the fluctuations for the transition from dissipative structures to order (I. Prigogine). In the paper (Vestn. Leningrad Univ. 1991, ser. Physics, n. 25, P. 38-43), Prudnikov and Shapkina have proposed the description of the processes of self-organization on the fluctuation level. According to this criterion the level of self-organization of natural process may be presented by the following manner:

$$L_s = [l_o^2 + (k_d + 2RAl_o)S_in + A^2S_i^2n^2 + k_kS_i^3n^3 + k_nS_i^4n^4]^{1/2} \qquad (1)$$

Where L_s is the absolute level of self-organization of the given natural process, or the random fluctuations in this process; l_o is the zero level of self-organization, or the fluctuations for other processes of this system; S_i is the sensitivity of the process to the different influences, or the instability of the process, which is determined by the theory of the examined natural process and includes the flow of the energy in the system; n is the scale of the process, which is characterized by the quantity of the substance in this process or the substance concentration; k_d, A, k_k and k_n are the coefficients of the individual levels of the self-organization; R is the coefficient of the co-correlation. According to the equation (1), the value of S_i^{-1} determines the stability of the system in the conditions of the different influences. The equation (1) demands to observe the five levels of the fundamental relations and the states for the natural processes. These levels are connected with the stability of the process and its energy in the power 0, ½, 1, 3/2, 2. The first three terms on the right-hand side of above expression characterize the linear range of the dependence of the parameters of the process from the energy and scale of the process and system, whereas the following two terms determine the non-linearity with the change of the scale of the system.

One can distinguish the five basic levels of the conditions of the substance: submicro up to elementary particles; micro up to atoms; the linear conditions of the environment up to planets; the nonlinear world from stars up to black holes and hyper nonlinear world up to great explosion. The each natural process has also the five levels of the passing from zero up to stochastic, linear, nonlinear and catastrophic level. In reason of this the development of any process from space to life passes of the stochastic, linear and nonlinear stages in the dependence of the energy and the scale of the system, and is finished the transition in new condition of the system or the catastrophe. The evolution is the continuous chain of the development process from space up to intelligent life. The time (t) is the function of the function of the speed of the process passing: $t=F(S_in)= F(L_s)$ (2). The quantitative characteristic of the self-organization processes and their comparison may be realized most effective by use of the relative value of the level of the self-organization (L_{sr}):

$$L_{sr} = [l_o^2 S_i^{-2} n^{-2} + (k_d + 2RAl_o) S_i^{-1} n^{-1} + A + k_n S_i n + k_k S_i^2 n^2]^{1/2} \qquad (3)$$

The expression (3) allows comparing the any natural processes according to the self-organization level independently the type and the theoretical basis of the processes. Here the time is connected with coefficient **A**, and the time is one order of the magnitude for any natural process. The theory allows tracing the evolution from space to life, from the simple systems up to complex systems, from to biological matter up to intelligent life. According to these positions the theory have not only the scientific importance, but the theory may play the essential philosophical role.

ON THE ROLE OF MOLECULAR SPACE AND TIME ASYMMETRIES IN THE ORIGIN OF LIFE

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In the lecture we shall explore the role of the fundamental symmetries of physics in the molecular origin of life – in particular the space, time and matter – antimatter symmetries expressed in C, P, T symmetries and their combinations (CP, CPT). In particular, molecular and biomolecular chirality are related to these symmetries and may be considered to be molecular "fossils" of evolution. The two key concepts here are the tunnel effect (introduced by F. Hund for the stereomutation of chiral molecules in 1927 [1]) and the influence of the electroweak parity violation suggested already by Yamagata in 1966 to be of potential relevance for biomolecular chirality [2]. In the lecture we will mainly report about the recent efforts of the Zürich group related to the theoretical discovery (in 1996 [3]) that parity violating electroweak potentials are orders of magnitude larger than previously calculated. We will provide the general theoretical background [4-6] as well as recent applications [7-10]. We shall mention current spectroscopic efforts on molecular parity violation [11-13], as well as possible conclusions to be drawn for the biomolecular evolution of life [14-16].

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ON CHARACTERIZATION OF 2-D PROTEOMICS MAPS

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Proteome has been defined as the totatlity of all proteines in cells of particular organ or tissue of living systems and proteomics research is concerend with identification, characterization, quantification and the study of interaction and function of proteins in a cell. Fromally proteome is defined as PROTEin complement expressed by genOME (or tissue). The challenge is due to complexity of cells that typically contains thousands and thousands of proteins. Proteomics map is obtain by separating proteins by charge (electrophoretically) and by mass (chromatographically) on a 2-D gell. Such 2-D maps have been, and continue to be, examined mostly visually. I will review recent development of quantiative (numerical) approach for comparison of different 2-D maps based on construction of sets of map invariants, which are themselves obtained by associating with a 2-D map matrices based on embedded curves and embedded graphs (based either on partial ordering of protein spots by charge and mass, or based on clustering of spots which are at small distances. Numerical characterization of proteomics maps is viewed by some as potentially a major breakthrouh in the proteomics research.

Although a characterization of 2-D proteomics maps is considering just one of many aspects of the proteomics research it is likely to help in answering other complex problems, including the study of the function of interacting proteins within a single cell. The question "Where do we come from and where are we going to?" relating to Life on a macroscale may well benefit from the question "Where do we come from and where are we going to?" relating to Cells on a microscale - which is the central question to the Proteome Research.

SOLAR INFLUENCE ON CLIMATE

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More and more studies indicate that variations in solar activity have had a significant influence on Earths climate. In spite of many ideas and much effort, the mechanisms responsible for solar influence on climate is still not known. One possibility is to influence the atmospheric transparency by changing cloud properties via cosmic ray ionisation (the latter is modulated by solar activity). Support for this idea is found from satellite observations of cloud cover. Such data have revealed a striking correlation between the intensity of galactic cosmic rays (GCR) and low liquid clouds (< 3 km). GCR is responsible for nearly all ionisation in the atmosphere below 35 km. One explanation could involve ion-induced formation of aerosol particles (0.001-1 mu in diameter) that can act as cloud condensation nuclei (CCN). A systematic variation in the properties of CCN will affect the cloud droplet distribution and thereby influence the radiative properties of clouds. If the GCR/Cloud link is confirmed, variations in galactic cosmic ray flux, caused by changes in the solar activity could influence Earths radiation energy budget. In particular the magnetic flux carried by the solar wind has more than doubled during the last 100 years, at the same time as the global temperature has risen.

LIPID VESICLES AND THE ORIGIN OF SOME CELLULAR PROCESSES

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Lipid vesicles are macroscopic objects defined by a lipid membrane enclosing an aqueous medium and separating it from the external aqueous medium. The division of space into internal and external compartments is also the basic characteristic of living cells. Lipid vesicles can form spontaneously and as such they may have been one of the important basic structures involved in biogenesis. Lipid vesicles also possess a variety of properties which could have been employed in the further evolvement of biological systems. Here it is argued that the cellular processes which involve changes of membrane conformations have their origin in the general shape behavior of closed lamellar membranes. This notion is based on some general features of the vesicle shape behavior which are the consequence of the layered membrane structure and do not depend on the structural and compositional details of the composing monolayers. One can thus ascribe these features also to prebiotic vesicles, even without knowing from what type of lipids they were made. The two general features of vesicle shape behavior that may be particularly important bases for possible physical mechanisms underlying different cellular processes are the symmetry breaking in vesicle shape transformations and the propensity of lipid vesicles for budding. The occurrence of stable asymmetric vesicle shapes is proposed to represent the mechanical origin of cellular polarity, and through this also of the biological order. Membrane budding is an obligatory step in vesicle fission and fusion processes taking place in cellular membrane trafficking. At the phenomenological level certain aspects of all these processes can be interpreted already on the basis of the understanding of the shape behavior of lipid vesicles. However, lipid vesicles and cellular systems differ in that the processes involving vesicles are in general stochastic, whereas the processes in a cell are based on a complex protein machinery and are in general deterministic. The point is made that some cellular processes, notable examples are cytokinesis, endocytosis and exocytosis, still emerged from the corresponding physical processes occurring also at the level of pure vesicles, but were properly upgraded and became well regulated in the course of evolution.

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NEW INTERSTELLAR AND LABORATORY MOLECULES

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Over the past five years, 130 new molecules have been discovered in our laboratory, in support of an observational program to identify and characterize new molecules in space. Most of these new species are highly reactive carbon chains -a type of molecule known to form readily and survive in the harsh, ultra-low-density environment of the interstellar gas--but a significant fraction are rings, or rings attached to carbon chains, and a number contain the hetero atoms N, O, S, and Si. On the basis of our laboratory frequencies, at least 7 of these molecules have already been identified in our galactic system in interstellar molecular clouds or circumstellar shells, and it is likely that many more will be detected during the next few years with the operation of powerful radio telescopes now under construction. The use of Fourier Transform Microwave Spectroscopy in the radio band, and laser Cavity Ringdown Spectroscopy in the optical, which yielded the new molecules will be described.

DIFFRACTION OF MATTER WAVES FROM NANOSTRUCTURES: NEW PHYSICS AND NOVEL APPLICATIONS

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Recent nanotechnology advances have made it possible to produce free standing transmission gratings with slits of 50 nm width. The diffraction of atoms, molecules and small clusters from such gratings provide beautiful textbook examples of matter wave phenomena [1]. Since only the wave nature of the particles is involved even the exceedingly weakly bound He dimers (binding energy $\approx 10^{-3}$ K ($\cong 10^{-7}$ eV)) and other small He clusters with up to 26 atoms can be separated by virtue of their different de Broglie wavelengths. Deviations of the diffraction intensities from predictions by traditional optics have been used to measure for the first time the long range particle-surface potentials [2] and the geometrical sizes of the He dimer ($\approx$ 50 Å) [3] and of the trimer (10 Å).

With three identical transmission gratings a Mach-Zehnder universal matter wave interferometer has been demonstrated. This device opens up a wide range of intriguing new experiments in molecular physics and has long range implications for studying decoherence as predicted by modern quantum theories of gravity. Transmission Fresnel zone plates have also been used to focus an atomic beam onto a 1 micron diameter spot [4], so that an essential part of a uniquely surface sensitive atom microscope is now available.

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NEW SYMMETRIES FOR FULLERENES: NEW TOOLS FOR THE DESCRIPTION OF CARBON ONIONS AND CARBON NANOTUBES.

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Using some simple geometric arguments it is explained how a new mathematical tool - an affine extension of noncrystallographic Coxeter groups - can be used to construct models which describe the location of atoms in fullerenes such as Carbon onions and Carbon nanotubes. We display the point sets obtained in our models and compare with existing results. Background in group theory is not expected - all concepts will be introduced and implemented on a purely geometric level.

CURRENT IDEAS ABOUT THE FIRST CELLS AND THEIR PRECURSOR STRUCTURES

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Nobody knows how life originated and whether it originated on Earth or somewhere else. Since today's living systems - including simple unicellular bacteria - are all very complex, it is rather difficult to understand how a living system could originate from the non-living. Although there are a number of experimental data on the synthesis of biologically relevant molecules carried out under presumably prebiotic conditions, it is difficult to imagine how the first cell(s) formed as a result of a prebiological, chemical evolution. It may well be that the ideas about the origin of the first cells do not consider all the possibilities which are given by the self-organization of amphiphilic molecules, compounds which have water-soluble as well as water-insoluble parts in their molecular structure. In addition to the obvious role of certain amphiphiles in the formation of the lipid matrix of the cell membrane, there may be other important roles of amphiphiles to be considered. Some of these possible roles are discussed.

HIGH-PRESSURE CESIUM DISCHARGE LAMP

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High-pressure sodium sources of light have been spread all over the world despite the fact that color reproduction is relatively low. In addition, because of small amount of mercury in the discharge plasma, there is an environmental problem with the poisoning effect of the soil where the old lamps are stored.

In search for a better and nontoxic new light source we received pulsed high pressure cesium lamps of 80 Watt power. Color rendering index of this high-pressure cesium lamp is more than 95 (class 1A). In a usual pulsed regime the visible spectrum can be approximated with a Planck function for black body radiation at 3800 K [1,2]. Unfortunately, the efficiency of this high-pressure cesium discharge lamp has reached only 50 lumen/watt. We believe that the main cause of this might be a considerable loss in the infrared spectral region. Thus, the present application of high pressure pulsed cesium discharge lamp as a new light source is precluded.

The goal of a present research is to analyze spectra near UV, visible and infrared regions, in order to perform lamp tailoring with our knowledge of spectral phenomena in alkali plasmas [3-5]. We also believe that a few technical modifications are required to make this source of light more efficient. The new results will be presented and discussed.

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