ON FRIES AND CLAR STRUCTURES IN PREDICTING π–RESONANCE ENERGIES OF BENZENOIDS

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We investigated benzenoids with five, six and seven rings. A correlation between π–electron resonance energies DRE and TRE and number of Kekulé structures in these molecules has been studied. We tried to improve the correlation by taking also into account Fries and Clar structures.

STUDY ON MATURITY OF FINITE GROUPS *via* APPLICATION IN MOLECULAR SCIENCE

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THE WIENER AND DETOUR INDICES OF NANOSTARS

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A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. The aim of this talk is to report our recent results on the problem of computing Wiener and detour indices of these new nanomaterials.

Keywords: detour index, nanostar dendrimer, Wiener index

ISOLATION OF A CHEMOLITHOTROPH ACIDOPHILIC BACTERIUM OF QOTOURSOU SPRING IN ARDEBIL PROVINCE FOR USING IN BIOLEACHING

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Continues extraction of mines has caused lack of storage. For solving this problem, we need effective process for exploitation of ores with low rover. Nowadays the microbial leaching technology is used for extraction of valuable metals from ores with low rover. For this purpose we isolated a strain of gram–positive chemolithotroph acidophilic bacteria from mineral acidic and sulphuric water of Qotoursou Spring in Ardebil Province. Bacterium has the optimum growth at 50^{o} C and pH = 3. It is able to oxidate ferrous iron, elemental sulphur, thiosulphate and iron sulphide and as a result of oxidation, ferric iron sulphate is obtained. This process of the intense oxidation is of great importance in extracting metals from sulphide ores. In this study, bacterium, grown in a culture containing ore samples from Sarcheshmeh Copper and Gendy Gold Mines, oxidized insoluble copper in chalcopyrite to copper sulphate soluble in water.

Keywords: acidophilic, chemolithotroph, leaching, microbial, Qotoursou spring

CLAR STRUCTURES: GRAPHENE, CYCLACENES, CYCLOPHENACENES, FULLERENES, NANOTUBES, NANOCONES, AND NANOTORI

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A finite portion of a graphene sheet with Clar sextets can be raised from two dimensions to three dimensions by various operations affording 3D–structures such as nanotubes, nanocones, or nanotori, and if pentagons are allowed to be included, also fullerenes can result. If after such operations the overlapping Clar sextets coincide, then special properties of the congruently—folded 3D structures become manifest. In geometrical terms, the product of the operation (*i. e.*, the 3D–structure) and its properties depend on two integer vectors h and k ($h \geq k$) and their difference $m \equiv h - k$ (modulo 3). The analysis encompasses graphene, cyclacenes, cyclophenacenes, fullerenes, nanotubes, nanocones, and nanotori.

APPLICATION OF WAVELET NEURAL NETWORK IN SIMULTANEOUS DETERMINATION OF IODATE AND PERIODATE BY KINETIC SPECTROPHOTOMETRY

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A kinetic spectrophotometric method for the simultaneous determination of iodate and periodate in mixtures was proposed. The method is based on the reaction of periodate and iodate with pyrogallol red in sulphuric acid media. The reaction was monitored spectrophotometrically by measuring the decrease in absorbance of pyrogallol red at 470 nm. Kinetic data collected at 470 nm, were processed by principle component artificial neural network (PC–ANN) method. The constructed model was able to predict the concentration of two species in the range of 0.1–15 and 0.1–17 μg/ml for iodate and periodate, respectively. The proposed method was applied for the simultaneous determination of iodate and periodate in several real samples with satisfactory results.

Keywords: iodate, periodate, pyrogallol, PC–ANN, spectrophotometry

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RECURSIVE NEURAL NETWORK MODELLING OF BENZENE DERIVATIVES ACUTE TOXICITY

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A data set containing acute toxicity values (96–h LC_{50}) of 69 substituted benzenes[1] for fathead minnow (*Pimephales Promelas*) was investigated by a Quantitative Structure–Activity Relationship (QSAR) model based on Recursive Neural Networks (RNN).[2] This model derives a QSAR from the direct treatment of the molecular structure, described through an appropriate graphical tool (variable–size labelled rooted ordered trees) by defining suitable representation rules.[3, 4] The input trees are encoded by an adaptive process able to learn, by tuning its free parameters, from a given set of structure–property training examples. Due to the use of such flexible encoding approach, the model is target invariant and does not need any a priori definition of molecular descriptors.
A comparative study between the results obtained by RNN–QSAR and Multi–Variant Regression methods[5] was carried out.

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THEORETICAL STUDY OF 1,3-DIPOLAR CYCLOADDITIONS OF PHENYL AZIDE WITH DIFFERENT OLEFINS USING DFT–BASED REACTIVITY INDEXES

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The 1,3–dipolar cycloadditions of phenyl azide with a variety of olefins have been studied by means of density functional theory (DFT) method. These results derived from the theoretical calculations shown that the concerted mechanism is both kinetically and thermodynamically preferred. The comparison of the calculated results between the 1,3–dipolar cycloadditions of phenyl azide with electron–deficient olefins and electron–rich ones is employed. The calculations have been done in the B3LYP/6-31G* level in gas phase. We led a theoretical study while being based on the following theoretical approaches: the theory of the transition state, the calculation of the activation energy, and the DFT–based reactivity indexes.

Key words: DFT–based reactivity indices, DFT calculations, orbital molecular theory, regioselectivity, 1,3–dipolar cycloadditions

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MICROWAVE CATALYSIS: THEORY VERSUS SIMULATION

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In this contribution we propose a novel physical mechanism for microwave catalysis based on rotationally excited reactive species and verify its validity through a computer simulation of a realistic chemical reaction–neutral ester hydrolysis. This nonequilibrium system is formally described by introducing rotational temperature, which is higher than the translational temperature. A Born–Oppenheimer surface was constructed on the density functional theory level and applied to a modified Monte Carlo scheme. The simulation gave a reduced activation free energy when the rotational temperature was higher than the translational temperature, which constitutes a catalytic effect. For example, our simulation predicts that with rotational and translational temperatures of 310 and 300 K, respectively, the reaction should proceed 4.5 times faster than when both temperatures are 300 K. Moreover, this microwave catalytic effect is less pronounced at higher temperatures, which may have serious implications for the interaction of microwaves with living organisms in the context of widespread mobile telephony. The simulated results will be compared against an analytical model, which is being developed to address the issue of microwave catalysis.

POTENT CARCINOGEN AFLATOXIN B$_1$: INHERENT STEREOSPECIFICITY AND EFFICIENCY OF DNA CATALYSIS

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Kinetic analysis of guanine alkylation by aflatoxin B1 *exo*–8,9–epoxide, the reactive form of the hepatocarcinogen aflatoxin B1, shows the reaction to be > 2000 times more efficient in DNA than in aqueous solution, that is, with free 2'–deoxyguanosine. Thermodynamic analysis reveals AFB1 *exo*–8,9–epoxide intercalation as the predominant source of the observed DNA catalytic effect. However, the known *exo* > *endo* epoxide stereospecificity of the DNA alkylation is observed even with free deoxyguanosine (ratio > 20:1 determined by LC–MS and NMR measurements), as beforehand predicted by our theoretical calculations. The evolutionary origin of the observed DNA catalytic effect will be discussed.

NANOCONES
A CLASSIFICATION RESULT IN CHEMISTRY

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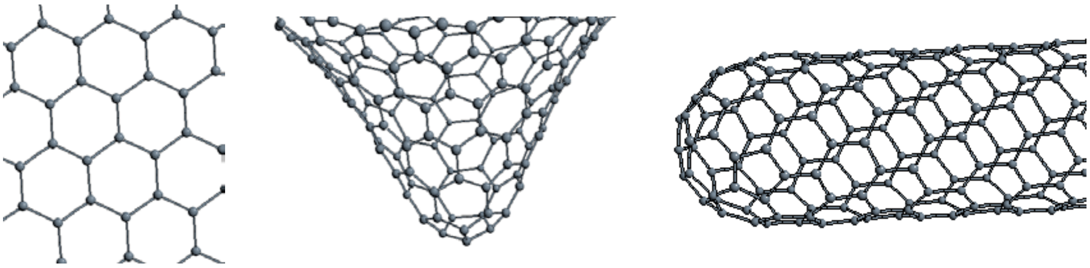
Nanocones are carbon networks conceptually situated in between graphite and the famous fullerene nanotubes. Graphite is a planar carbon network where each atom has three neighbours and the faces formed are all hexagons. Fullerene nanotubes are discussed in two forms: once the finite, closed version where except for hexagons you have 12 pentagons and once the one–side infinite version where 6 pentagons bend the molecule so that an infinite tube with constant diameter is formed. A nanocone lies in the middle of graphite and one–side infinite fullerene nanotubes: next to hexagons it has between 1 and 5 pentagons, so that neither the flat shape of graphite nor the constant diameter tube of the nanotubes can be formed. Recently the attention of the chemical world in nanocones has strongly increased. The figure below shows an overview of these types of carbon networks.



The structure of graphite is uniquely determined, but for nanotubes and nanocones an infinite variety of possibilities exist. There already exist fast algorithms to generate fullerene nanotubes (see Ref. 1) that are *e.g.* used to detect energetically possible nanotubes.

In this talk we describe a classification result and a generator for nanocones.

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NEW FEATURES OF THE SYSTEM CHEMOGRAPHIX

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The authors recently obtained a characterization of matrices $M = \{m_{ij}\}$, such that there exists a graph $G = (V,E)$ with m_{ij} equal to the number of edges with end degrees i and j in G. It was observed that for chemical graphs and given numbers n of vertices (and possibly m of edges), the feasibility problem for G can be expressed as a mixed integer program without an objective function. It was also observed that a large variety of chemical graphs optimization problems were amenable to the same format. The only, but important, restriction is that the indices appearing in the objective function depend only on the degrees of the vertices of G.

Based upon this characterization, the CGX system was build. In its current version, CGX handles the Randić index and most of its extensions (generalized Randić index, zero–th order Randić index), the Zagreb indices, the variance of degrees and the discrepancy among others. As the resolution of the mixed integer program underlying CGX is very fast and regardless the number of vertices or edges of the graph, the system may be used in a parameterized manner (for various values of n, m and possibly another variable) and provide a large number of extremal solutions.

A numerical method using linear programming is now implemented in CGX to summarize information from the obtained solutions and derive conjectures. This method may be used to find bounds on the objective function, but also to characterize the extremal graphs obtained by the system. We will present the latest version of the system and some results obtained by its means.

WIENER INDEX ON FRACTAL SIERPINSKI 2–D INFINITE LATTICE

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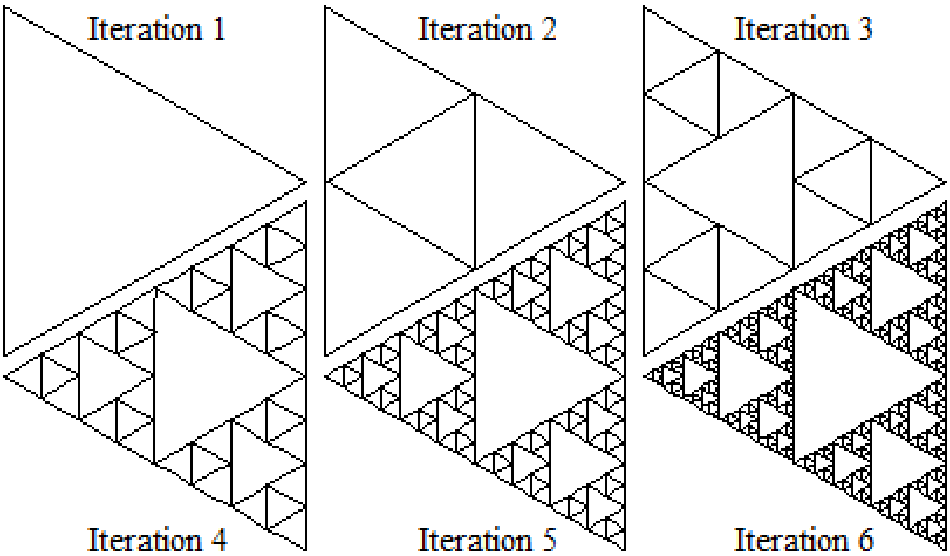
Recently, we introduced a relevant conjecture for the Wiener index of infinite periodic lattices: for dimensional infinite transitionally invariant lattices generated by a unit cell with n_0 atoms, where L number of unit cell atoms along edges (*e.g.* the lattice is made of $L^{d}{}_{T}$ cells), the Wiener index of the is exactly determined by a lattice–specific polynomial in L of degree $\underline{k} = (2d_T + 1)$, and thus W(N) with $N = n_0L^{d}{}_{T}$.

In this presentation we compute the Wiener index for planar Sierpinski lattices, documenting the first extension of above conjecture to non–periodic infinite lattices. Being N the number of nodes of the Sierpinski graph after t growing steps (at initial step t = 1, N = 3, W = 3), the relationship $W(N^{\underline{s}})$ has been derived on the basis of above conjecture. Dimensionality implications of leading exponents are also discussed. Moreover our computations produce extended evaluations of average eccentricity of Sierpinski graphs.



THE EFFECT OF LIGHT ON THE COMPOSITION OF SOME VOLATILE COMPOUNDS IN WINE: AN HS–SPME–GC–MS STUDY

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Solid phase microextraction (SPME) is a valid instrument to determinate volatile organic compounds.

Some years ago, Benitez *et al.* (2003) reported that the UV–vis irradiation of Sherry wine provokes an increase of volatile compounds. These results are not in agreement with those of D'Auria *et al.* (2003) where SPME was used in order to estimate the modifications occurred in volatile compounds in champagne after UV irradiation. In this case, in fact, authors observed a sharp reduction in the amounts of esters. Considering that the esters are important constituents of the aroma of wine, it is obvious that it can be influenced in both cases.

Furthermore, Benitez *et al.* (2004) showed that also the nature of the glass of bottles is important element for organoleptic properties of wine. The increase of esters was higher in topaz glass than in a transparent one.

For these reasons we decided to study the irradiation of a white wine (*Fiano di Avellino* – Campania) and a red one (*Aglianico del Vulture* – Basilicata). We performed the irradiation with a low pressure mercury arc by using Pyrex glass in order to understand the photochemical behaviour of wine in controlled conditions and in the original bottles to simulate the real exposition of wine to light.

We observed a rapid photodegradation of volatile compounds in both wines. In particular we observed degradation of both alcohols and esters (in agreement with what reported from D'Auria *et al.* (2003) about champagne but not with results of Benitez *et al.* (2003) about red wine). This incongruence can be explained considering that also in our studies the amount of esters was increasing in the red wine after 2h of irradiation. Only for longer times we observed the degradation of these compounds.

These behaviour can be explained assuming the presence of a protecting agent in red wine that is destroyed by light and assuming that light can increase the amount of esters through a Norrish type II reaction from a suitable precursor (Hermann, 2007).

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MODIFIED THOMSON PROBLEM

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The modified Thomson problem, which concerns an assembly of N particles mutually interacting through a Coulombic potential and subject to a Coulombic–harmonic confinement, is introduced. For sufficiently strong confinement strengths M, properties of its solutions (such as the energy and the particle positions at the minimum, and the corresponding zero–point vibrational energy) are accurately estimated by expressions dependent on only a few quantities pertaining to the original Thomson problem [such as the energy $E_{Th}(N)$] and the reduced confinement strength $\xi = N M / E_{Th}(N)$. For $N \leq 12$, this regime of the perturbed Thomson problem persists for all non-negative values of ξ. On the other hand, the perturbed spherical Coulomb crystal regime emerges for $\xi < \xi_{crit}(N)$ and larger numbers of particles. For $13 \leq N \leq 22$, the transition that delineates these two regimes is due to the existence of two energy minima, the crystal-like one becoming global for sufficiently weak confinements. For $N \geq 23$, the transition involves a catastrophe brought about by the vanishing of one of the Hessian matrix eigenvalues, the value of $\xi_{crit}(N)$ being related to the magnitude of radial instability in the corresponding solution of the original Thomson problem.

MATHEMATHICAL METHODS IN ANALYZING OF GROWTH REGULATION IN MAMMALIAN EMBRYO IN CHEMICHALLY DEFINED MEDIUM *in vitro*

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The modified organ culture method devised in our laboratory is a very successful model for investigating growth of mammalian embryos developed in teratoma–like explants, built of intermixed tissues. During embryonic development a number of drugs act on growth regulation as well as on differentiation. In this research we investigated the growth of mammalian embryos cultivated in chemically defined medium *in vitro*, in response to fibroblast and nerve growth factors (FGF and NGF) and their possible synergistic action. Both agents modulate biological effects ranging from neuronal differentiation and survival like NGF, to proliferation, migration, tissue regeneration, wound healing like FGF, and they are important factors in the pathology of different human illness. Biological activity of FGF and NGF has been also established in embryo growth as well as in the grown organisms. Both proteins affect genes via specific receptors, and their mitogenic or antimitogenic activity depends on the type of cell differentiated in developed teratomas.

We treated rat gastrulating embryos with 100 ng/ml and 200 ng/ml of NGF or FGF, and with both agents combined in serum–free medium (MEM). Growth rate of explants *in vitro* was evaluated by measuring average size of explants using an eyepiece micrometer on a few particular days during 14 days of culture. The perpendicular major and minor diameters of each explant were measured and expressed as the arithmetic mean of those two values. Primary differences in size (arithmetic mean of two diameters) between explants disabled us to correctly analyze the influence of different factors simply by observing the size of explants. To avoid this problem, we calculated the changes in size of explants (expressed in percents) and then analyzed this information instead of the actual size. We estimated differences between respective groups using Student's t–test and our results were mathematically more accurate since now all the explants start from the same point (0% change).

Both concentrations of NGF impaired growth of explants, while FGF stimulated growth, although it was not always significantly different from control groups on a particular measure–day. When we applied NGF and FGF together in culture media the growth of explants was improved in comparison to control and experimental NGF–treated or FGF–treated groups. FGF reduced inhibitory effect of NGF, but it could not prevent it and significantly increase growth.

GLOBAL RANKING OF PHOTOCHEMICAL AIR POLLUTION MONITORING SITES

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The recent introduction of the photochemical pollution indicator (Cvitaš *et al.*, *Env. Monit. Assess*., in press) based on hourly averages of ozone concentration from long term monitoring allows to express photochemical site pollution by a simple number. Its application to 12 European ozone monitoring sites of the EMEP network yielded a reasonable rating with station Montelibreti near Rome airport as most polluted. Here we compare these results with those for three stations in Greater Baton Rouge (Louisiana, USA) and several stations from Pear River Delta around Guangzhou (China) which all are considered to experience considerable photochemical pollution.

INFORMATION MEASURES FOR CHARACTERIZING WEIGHTED CHEMICAL GRAPHS

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An essential part of QSPR (Quantitative Structure–Property Relationships) deals with converting chemical structures into molecular descriptors which are relevant to detect physicochemical or biological properties.[1] An important task in QSPR is to characterize chemical graphs by calculating their structural information contents.[2] For this, Shannon–Information measures representing entropies of the underlying graph topology have been intensely applied.[2] The major problem of the known information indices used in mathematical chemistry is that they operate only on unweighted graphs (skeletons), *i.e.*, all atoms and bonds are considered as equal. To characterize chemical structures more adequately than right now, we will propose a novel entropic measure that takes edge and vertex labels of the underlying graphs into account.

The theoretical basis for our investigation forms an information measure to determine the structural information content of unweighted and undirected chemical graphs.[3] By incorporating edge and vertex labels, we get certain families of information measures to quantify the structural information content of weighted chemical structures. As a result, our novel measures can be considered as a powerful generalization of the existing one that was presented in Ref. 3.

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TOPOLOGICAL CHEMISTRY

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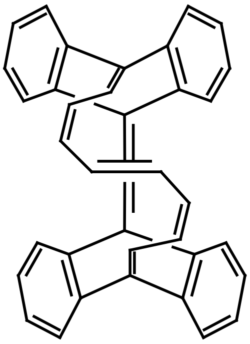
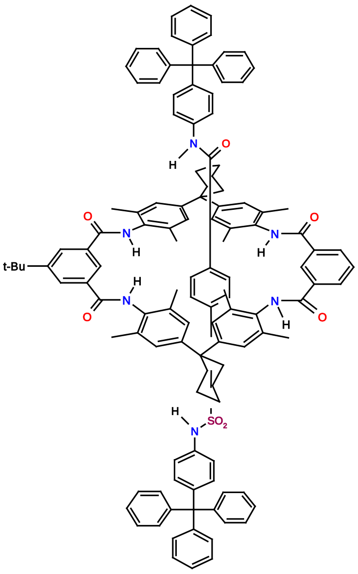
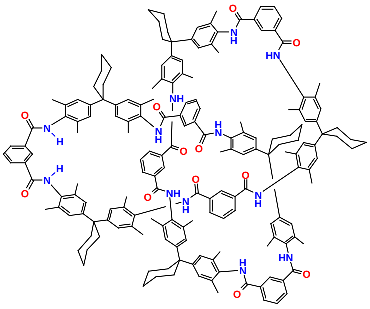
On the intersection of mathematics, chemistry and biology, topological chemistry[1] enables one not only to study such exciting molecules but we are also close to their commercial applications.[2,3] A fascinating story of their discovery and the development of the whole domain will be presented in brief. Molecules modeling links (catenanes), knots, Moebious strips and some other structures have been synthesized. To include the latter (*e.g.*, rotaxanes and endohedral fullerene complexes) the definition of distinct properties should be precized to describe real molecules differing from abstract mathematical notions.



Möbious strip



Rotaxane



Knot

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ECCENTRIC CONNECTIVITY INDEX

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Eccentric connectivity index has been found to have a low degeneracy and hence a significant potential of predicting biological activity of certain classes of chemical compounds. We review here basic mathematical properties of this index and present formulas for eccentric connectivity index of various families of graphs. We also show that a path and a star are extremal with respect to this index among all trees.

ON CYCLIC CONJUGATION IN FLUORANTHENE–TYPE POLYCYCLIC CONJUGATED HYDROCARBONS

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Fluoranthene and its congeners are compounds that, in view of their chemical and physical properties, are closely related to benzenoid hydrocarbons. Yet, because of the presence of the five–membered ring, the pattern of cyclic conjugation in fluoranthenes is somewhat different than in benzenoids. We studied cyclic conjugation in fluoranthenes by calculating the energy–effects of individual rings. By means of this method, we could establish several general regularities for the cyclic conjugation in fluoranthenes, especially for its five–membered ring.

SPECTRAL MEASURES FOR MOLECULES

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COMPUTING DISTANCE BASED TOPOLOGICAL INDICES OF NANOSTAR DENDRIMERS

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A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. The aim of this paper is to present our latest results on the problem of computing distance based topological indices of nanostar dendrimers. Our method is general and can be applied for graphs containing separate cycles.

Keywords: dendrimer, distance based topological index, nanostar

FOUR GENERALIZATIONS OF COLUMN–CONVEX POLYOMINOES

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There are three regular tilings of the Euclidean plane: the triangular tiling, the square tiling, and the hexagonal tiling. We adopt the convention that every square or hexagonal tile has two horizontal edges. In a regular tiling, a tile is often referred to as a *cell*. A plane figure P is a *polyomino* if P is a union of finitely many cells and the interior of P is connected. So, chemically speaking, a polyomino with hexagonal cells is a possible benzenoid hydrocarbon.

We consider polyominoes P and Q to be equal if and only if there exists a translation f such that $f(P) = Q$.

Given a polyomino P, it is useful to partition the cells of P according to their horizontal projection. Each block of that partition is a *column* of P. With this definition, a column of a polyomino is not necessarily a connected set. On the other hand, it may happen that every column of a polyomino P is a connected set. In this latter case, the polyomino P is called a *column–convex polyomino*.

Let a_n denote the number of those square–celled column–convex polyominoes which have n cells. It has been known at least since 1956 that the sum $a_1q + a_2q^2 + a_3q^3 + \ldots$ (called the *area generating function* of column–convex polyominoes) is equal to $\frac{q(1-q)^3}{1-5q+7q^2-4q^3}$.

Now, let a *column–duplex polyomino* be a polyomino whose columns can have either one or two connected components. Somewhat surprisingly, an exact enumeration of column–duplex polyominoes by area (in the sense of finding the area generating function) appears to be impossible. Hence, we are focused on models which interpolate between column-convex polyominoes and column-duplex polyominoes. We have defined altogether four such models: *cheesy polyominoes*, *polyominoes with cheesy blocks*, *column–subconvex polyominoes* and *simplex–duplex polyominoes*. In the first three models, the definition requires (perhaps among other things) that the gap within a two–component column must not be greater than m cells in size, where m is a positive integer which we set in advance. In the fourth model, the gap within a column can be of any size, but it is not allowed that two two–component columns come one immediately after the other.

Using the popular column–by–column technique (which originated in the work of Temperley and was further developed by Bousquet–Mélou and Svrtan), we computed altogether nine new area generating functions. The simplest one is the area generating function for $m = 1$ cheesy polyominoes with hexagonal cells: it is given by $\frac{q(1-3q+q^2)}{1-6q+8q^2-q^3}$.

The other generating functions (including some extremely complicated ones) can be seen on author web page: `http://www.gradri.hr/?rijeka=staff,43`

THEORETICAL ASPECTS OF FULLERENE CHEMISTRY

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Fullerene chemistry and physics is an area where three–way interaction between chemistry, mathematics and computer science is particularly strong. In these lectures, some applications of chemical graph theory will be discussed for these chemically important polyhedral all–carbon molecules, with emphasis on the way that understanding of trends can be obtained with the simplest of theoretical tools.

Systematics of fullerene physics and chemistry can be developed using a mixture of symmetry, combinatoric and graph theoretical arguments. Adjacency matrices and their eigenvalues (at least partially) characterise stability and reactivity of the unsaturated fullerene carbon frameworks, through the Hückel model. Isomer counts, magic numbers in electronic structure, energetics and patterns of addition chemistry can all be understood with the help of symmetry/graph theory based models. Discussion of the fullerenes can also be used as a way of learning more about these simple but powerful techniques. All the ideas and models used will be introduced *from scratch* , so that no specialised background knowledge will be assumed.

The main reference used will be *An Atlas of Fullerenes* by P.W. Fowler and D.E. Manolopoulos, which was first issued by Oxford University Press in 1995 and is now available in a cheap reprint form as a Dover paperback (ISBN 0–486–45362–6).

NOVEL VERTEX–DEGREE–BASED MOLECULAR STRUCTURE DESCRIPTORS

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Topological descriptors based on end–vertex degrees of edges in a graph have been studied more than three decades. Even today, they attract much attention especially of theoretical chemists. A number of such descriptors were introduced in chemistry. Maybe, the most employed and investigated is Randić connectivity index.

The atom–bond connectivity index (*ABC*) was introduced ten years ago by E. Estrada *et al*. Their main goal was to decrease the dependence of Randić index on branching. The *ABC* index is defined as follows:

$$ABC(G) = \sum_{uv=e\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \qquad (1)$$

where d_u and d_v are the end–vertex degrees of an edge e in a graph G.

In the seminal paper, authors had shown that the *ABC* index can be used as a useful tool in QSPR/QSAR researches.

Recently, the geometrical–arithmetic index (*GA*) has been introduced. The *GA* index is also based on end–vertex degrees. It is defined in a following manner:

$$GA(G) = \sum_{uv=e\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \qquad (2)$$

Prediction of the *GA* index has been tested on various physico–chemical properties. It has shown a reasonable prediction power in the case of some physico–chemical properties.

Here, these two indices are investigated in the case of benzenoid hydrocarbons and phenylenes. The exact formulas for calculation of *ABC* and *GA* indices of benzenoid hydrocarbons, as well as of phenylenes are found. Even more, the relation between *ABC* indices of benzenoid hydrocarbons and phenylenes is established. The similar relation between *GA* indices of benzenoid hydrocarbons and phenylenes is presented here.

COMPUTING THE MARKARACTER TABLE OF SOME NANO STRUCTURES

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The concept of markaracter tables of finite groups was introduced first by a Japanese chemist Shinsaku Fujita.[1–4] He applied this notion in the context of stereochemistry and enumeration of molecules. In this paper, a simple computational method is described, by means of which it is possible to calculate the markaracter tables of finite groups.

Keywords: fullerene, Mark Table, Markaracter Table, USCI Table

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THE INTEGER–VALUED CHARACTERS OF TETRA-BUTYL ALCOHOL

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In order to enumerate isomers of fluxional molecules, some definitions like maturity and the integer–valued characters of a finite group were introduced.[1-7] The full non–rigid group of tetra–butyl alcohol was introduced in Ref. 8.

In this paper, we introduce a new simple method to specify how a given finite group is matured or unmatured, and then, via GAP program[9], compute all the dominant subgroups and the integer–valued characters of the above molecule.

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TOPOLOGICAL COORDINATES FOR CARBON NANOSTRUCTURES

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Some eigenvectors of the adjacency matrix of spherical carbon structures produce satisfactory Descartes coordinates in a simple way. Namely the three bi–lobal eigenvectors with appropriate scaling produce the XYZ coordinates of the atoms. The idea can be generalized to toroidal structures as well. Here four bi–lobal eigenvectors of the adjacency matrix are needed in a geometric construction for calculating the coordinates. In the case of more complicated structures like junctions or helical tubes the generalization of this method is not trivial. We have developed a shape analysis for examining the possibilities to generate the topological coordinates for such kind of carbon networks as well. In the present talk we shall review our recent results on these topics and we shall present a method that is very promising for producing the topological coordinates for non-spherical carbon structures.

A NEW APPROACH IN TREATMENT OF CANCER

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Cancer is the result of an imbalance among cell cycle progression and cell death, what is a reason that cancer research is increasingly focused on cell cycle and cell death regulatory mechanism. Apoptosis is genetically controlled form of cell death, with a distinctive role in both the development and prevention of cancer. It could be induced by a variety of anticancer drug. It is now well established that the reduced capacity of cancer cells of undergoing apoptosis is the main point in the pathogenesis and progression of large number of neoplasis as well as in therapeutic treatment failure. A new approach in treatment of cancer is: specific targeted molecules and immunological treatment of cancer.

A great importance in the regulation of cell cycle progression, proliferation and apoptosis is the phosphatidylinositol–3 kinase – Akt (PI3K–Akt) signal transduction pathway. Over the last few years many studies have provided convincing evidence that constitutive activation of this pathway is involved in the aggressiveness and resistance to therapeutic treatments of a large number of malignant diseases. Accordingly, the deregulated activation of the PI3K–Akt survival pathway is often associated with hematological malignancies, including acute and chronic lymphocyte leukemia. Perfosine is one of the specific targeted inhibitor of Akt kinase. The most successful of the new generation of targeted anticancer drugs, in a limited group of patients, has been the tyrosine kinase inhibitor imatinib mesylate (glivec). This drug has major activity in chronic myeloid leukemia (CML), gastrointestinal stromal tumors (GIST), and some rare hematological and dermatological conditions. It is a specific inhibitor of tyrosine kinase formed by BCR–ABL fusion protein in CML.

Hyper proliferation of cancer cells is associated with deregulation of cell cycle progression, which is driven by the activities of CDKs. A key regulator of their activities is a p27 protein. It has significant role in cancer progression and antitumor drug response. To examine p27 as specific target molecule and its role in tumor cells apoptosis, protein transduction method is very suitable. Protein transduction could give an opportunity for delivering of drags into cells with emphasis on the specific target molecules. A protein p27 could be a suitable target for treatment of chronic lymphocitic leukemia (B–CLL). It is a currently incurable disease, characterized by accumulation of neoplastic B–cells, arrested in the early phases (G0/G1) of the cell cycle. The pathogenesis of the disease is largely unknown. Defective apoptosis and deregulation of some cell cycle regulatory genes/proteins may contribute to malignant process of B–CLL. An elevated level of p27 has been found in B–CLL. This protein plays an important role in the arrest of the cell cycle and in communication between the extracellular signals and cell cycle controlling mechanism.

Immunological treatment of tumors opened new therapeutic approach in the patients resistant to chemotherapy. In our hands, the influence of Rituximab (anti–CD20) and Campath 1H (anti–CD52) were examined on the samples from B–CLL patients. The results were compared with fludarabine, a known cytotoxic drug.

These examples are the model for targeting specific molecular markers of a cancer and give the promises that target inhibition can result in major clinical improvement.

THE STRONG–CORRELATION LIMIT OF FOUR ELECTRONS IN AN ISOTROPIC HARMONIC TRAP

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Asymptotically exact wavefunctions of the four–electron harmonium atom at the strong–correlation limit are given by Slater determinants multiplied by a Jastrow factor in the form of a single exponential function with the argument bilinear in the interelectron distances. The spinorbitals that enter the determinants set the multiplicities and angular momenta of individual states whereas the Jastrow factor fully accounts for the electron correlation. Asymptotically exact expressions for the corresponding electron densities, which can be computed from such wavefunctions with the help of the saddle–point approximation, have the form of products of Gaussian functions and polynomials in the Cartesian coordinates.

HISTORY OF MATHEMATICAL CHEMISTRY

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Mathematical Chemistry is a relatively new science, but its roots go far back into the past. In the lecture, among other (more recent) facts, we shall outline the following.

1. The oldest connection between mathematics and something that today we would include into chemistry comes from the Greek philosopher Aristocles of Athenes (427–347 B.C.), better known under his nickname Plato. Some fifty years before Plato, another Greek philosopher – Empedocles – proposed that the entire material world is made of four elements – fire, air, water, and earth. Plato studied regular geometric solids (nowadays known as "*Platonic solids*"). In that time it was established that there are exactly five such solids: tetrahedron, octahedron, icosahedron, cube, and dodecahedron. Plato claimed that fire is made of tetrahedra, air of octahedra, water of icosahedra, and earth of cubes. The remaining fifth polyhedron – the dodecahedron – was claimed to form the heavenly bodies.

Based on the fact that the faces of tetrahedra, octahedra, and icosahedra are triangles, whereas the faces of the cube are squares, Plato concluded that fire, air, and water may be converted to each other, but not converted to earth. This implied that melting of solids was not possible. Consequently, Plato concluded that metals such as iron, gold, copper, are not solids, but liquids.

This assertion of Plato may be considered as the very first result of Mathematical Chemistry, a result that is blatantly wrong.

2. Somewhere around the first century acted in Alexandria the chemist Cleopatra (a lady). In her "*recipe for obtaining gold*" we recognize an *ouroboros* – a tail–eating snake or tail–eating dragon. This was an ancient symbol for something that has no end, rather an endless algorithm than an infinitely (large or small) number. Pictures of *ouroboros*es are found abound in later alchemical writings.

3. The great medieval alchemist Jabir (Abu Musa Jabir ibn Hayyan, 721–815) in his "*Book of Metals*" claims that the numbers 1, 3, 5, 8, and especially their sum 17, are of great importance. According to Jabir, "*everything in the world is determined by the number 17*". Today we know that the scholars of that time were fascinated by the (then discovered) magic square:

4	9	2
3	5	7
8	1	6

They maintained that this magic square carries a concealed message from the God, which needs to be decoded. The numbers 1, 3, 5, and 8 are found in the lover left 2 x 2 block of the magic square. Why Jabir found them so important is today not known.

4. Medieval alchemists in Europe often used geometric constructions for trying to achieve the "*Great Work*" – transmutation of base metals into gold. This is best seen from pictures found in the books of Michael Maier (1618) and Daniel Stolcius (1624).

5. Alchemists used geometry for magical purposes. The first scholar who made mathematical considerations of the real (chemical) world may be Johannes Kepler (1571–1630), who in 1611 published a booklet "*Strena seu de Nive Sexangula*" (A New Year's Gift or the Six–cornered Snowflake). Kepler knew that snowflakes always have a hexagonal symmetry and meditated about the cause of this. From today's point of view, Kepler was very far from a true solution of the problem. Nevertheless, the use of geometry and symmetry in chemistry may have started then.

6. In his book "*Elements de la Philosophie de l'Art de Feu ou Chemie*" (Elements of the Philosophy of the Art of Fire or Chemistry), Paris, 1657, W. Davissone examined the shapes of various objects in nature (leafs, crystals, flowers, bee haves) and constructed simple geometric objects that looked similar to these. This is the true beginning of mathematical modeling in chemistry, especially by using geometry and symmetry (later: group theory). One can follow this through the entire later development of chemistry. We especially point out the tetrahedra of Jacobus van't Hoff (1874), which produced a revolution of stereochemistry.

7. Mikhail Vasil'evich Lomonosov (1711–1765) was a great Russian scholar, who – unfortunately – lived before the basic laws of chemistry, in particular Lavoisier's law of mass conservation, were discovered. In 1741 we wrote a text entitled "*Elementa Chymiae Mathematicae*" (Elements of Mathematical Chemistry), which he never published. This text was discovered only after Lomonosov's death. In it the name "*Mathematical Chemistry*" was used for the first time.

8. Until the second half of the 19th century chemistry was almost completely lacking mathematics. This motivated Immanuel Kant (in 1786) and Auguste Comte (in 1830) to give very negative opinions about chemistry. In particular, Kant maintained that chemistry is no science at all.

The lecture will not end at this point.

NAVIGATING A FOUR–DIMENSIONAL PERIODIC SYSTEM OF DIATOMIC MOLECULES

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The chemical elements, or atoms, may be enumerated by their atomic numbers Z. The obvious periodicity of their properties practically demands that we use period, or row, numbers R and group, or column, numbers C to form a flat chart of the elements. Compounds composed of diatomic molecules, or the diatomic molecules themselves, may be enumerated by the two atomic numbers (Z_1,Z_2) and can be arranged on the Z_1,Z_2 plane. Observations of data plotted on this plane show that they echo the periodicity of atomic data.[1] This is strikingly true of optical spectroscopic and high–energy cross–section data; it is somewhat more ambiguously true[2] of condensed-matter data. These observations invite us to use the atomic row and column numbers (R_1,C_1,R_2,C_2) as independent variables and to distribute the molecules in the R_1,R_2,C_1,C_2 hyperspace. (The bounds of this hyperspace conform to the shape of the chosen chart of the elements.) While navigating this space presents no obstacle to computers, we raise the question:

How shall we visualize where they lead us?

This presentation shows various aspects of a hypercube[3] and of the four–dimensional periodic system[4,5] containing all molecules except those with rare–earth atoms. Then we show planes containing all neutral molecules having:

(a) the #1 atom fixed,
(b) the #2 atom fixed,
(c) equal atoms, and
(d) a fixed number of electrons.

[Of course, what you see on–screen are three–dimensional objects, with optional perspective, that are projections of the four–dimensional objects (with optional perspective).]

But should the presentation be unclear or unpersuasive, there are more prosaic, three–dimensional, alternatives[5,6] that are *not* part of this presentation. We could:

(1) tile flat 118–element charts into rows and columns such that every chart contains all molecules having #1 or #2 atom appropriate to the row-column location in which it is laid;
(2) stack the flat 118 charts such that the centroid of each one lies above their atom #1 or atom #2 in a template periodic chart; or
(3) stack portions with fixed (R_1,R_2) or fixed (C_1,C_2) into piles, tori, or Möbius strips that may be arranged in order of one or more of these same four variables.

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ARTICLES IN METEOROLOGY AND ATMOSPHERIC SCIENCE JOURNALS: BIBLIOMETRIC ANALYSIS OF GLOBAL ATMOSPHERIC SIMULATION TREND

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Scientometrics is the quantitative evaluation of periodical literature that allows for the calculation of different indices characterizing and classifying scientific products. This study aims to evaluate the global scientific production of simulation research in the category of *Meteorology and Atmospheric Sciences* for the past 16 years and to provide insights on the characteristics of the atmospheric simulation research patterns, tendencies and methods that might exist in the papers, as well as in leading countries and institutes. Data were based on the online version of *Science Citation Index*, *Web of Science* from 1992 to 2007. Articles referring to atmospheric simulation were assessed by many aspects, including exponential regression fitting the trend of publication outputs with $r^2 = 0.9996$, distribution of source country, source institute, words in title, author keywords, and keywords plus, and four most cited articles within the years. By synthetically analysis of three kinds of keywords, it was concluded that atmospheric simulation research related on ***ozone***, ***climate***, ***circulation***, ***transport***, ***parameterization*** and ***assimilation*** was the orientation of all the atmospheric simulation research in the 21st century. Relevant researchers can realize the panorama of global atmospheric simulation research, and establish further research directions with the use of this new bibliometric method.

ROTATIONAL UNIT–DISTANCE REALIZATIONS OF I–GRAPHS

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We consider the question which *I*–graphs *I(n, j, k)* admit unit–distance representation in the Euclidean plane with an *n*–fold rotational symmetry. The answer to this question helps us determine the (Euclidean) dimension of several generalized Petersen graphs *G(n, k)*. Prisms, *G(n, 1)*, can be represented in this way only using degenerate unit–distance representations; however, since they are Cartesian products, it is easy to find a non–degenerate unit–distance representation (without rotational symmetry). It seems that the only generalized Petersen graph that cannot be studied using one of the two ways is the arc–transitive *G(12, 5)*. Unfortunately, there are some generalized Petersen graphs that admit rotational unit–distance realizations but result in various types of degeneracies.

RECENT PROGRESS OF Z INDEX IN NUMBER THEORY

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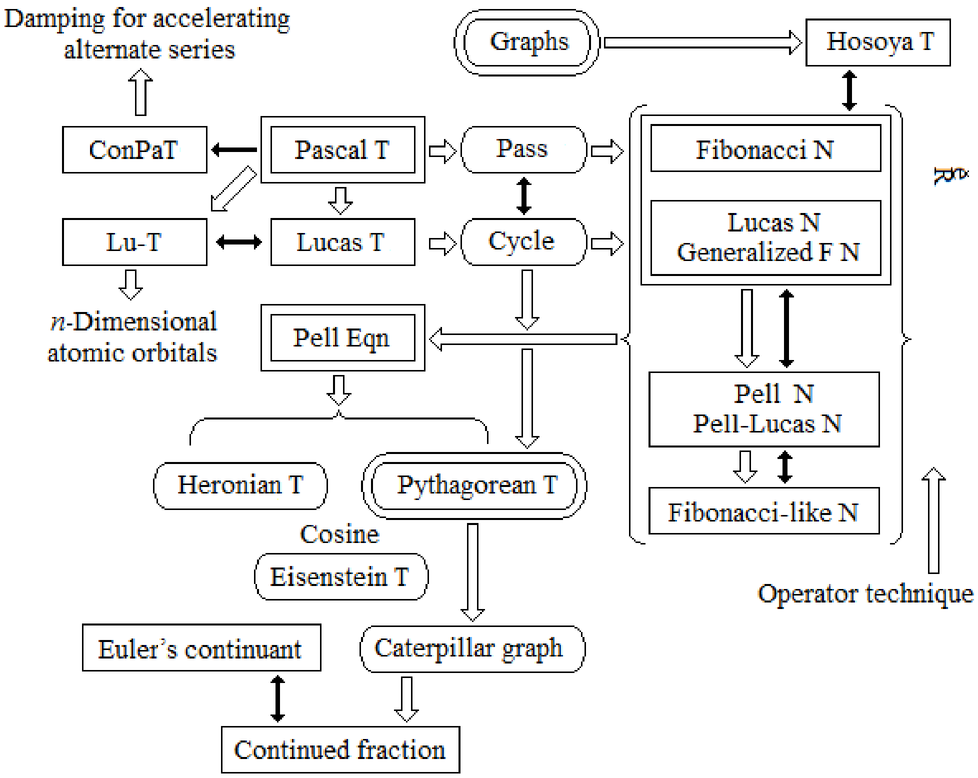
The topological index *Z* was proposed in 1971 originally for correlating the thermodynamic quantities of saturated hydrocarbons with the topological structure of their carbon atom skeletons.[1] Later it was extended to the graph–theoretical molecular orbital method for analyzing the topological dependency of the π–electronic structure and aromaticity of unsaturated hydrocarbons.[2] However, very recently it was found that my *Z* index has a very important role in number theory for providing proof technique and guiding tool by bridging between algebra and geometry.[3] Some of the results are illustrated in the diagram below. Several topics will be introduced in my lecture.



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APPROXIMATE GRAPH PRODUCTS

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The problem of computing approximate graph products was posed several years ago in a theoretical biology context by G. Wagner. The notion of a *character* (trait or Merkmal) can be understood as a property of an organism that in evolution can vary independently of other traits. Characters thus are not necessarily the same as observable properties such as arms, legs, fingers, a spinal chord, *etc*., although such observables of course often are instantiations of characters. The important biological distinction is whether such measurable attributes (or combinations thereof) form a *coordinate axis* along which the character states (*e.g.* the lengths of arms or fingers) can vary independently of other traits, or whether the underlying genetics dictates dependencies among the observables. We show that this question can be represented as a graph problem, where data are sampled from the observed phylogenetic transitions between many pairs of related species. Since the sampled information will always be incomplete and have limited accuracy we have to work with a graph representation of phenotype—space that will be known only approximately and that will cover only a limited region of interest. This forces us to consider an approximate and local theory. Given a graph G that approximately represents a phenotype space we reduce our task to finding a graph H that is a nontrivial strong product and a good approximation of G in the sense that H can be reached from G by a small number of additions or deletions of edges and vertices. Algorithmic solutions are of high complexity and lead to unfeasible computing times for the size of graphs we expect to treat.

Therefore our aims are fast, preferably linear, algorithms that recognize large classes of approximate graph products.

This talk describes the current state of the art in the recognition of approximate graph products.

*Joint work with:
Marc HELLMUTH, Werner KLOECKL, Tomas KUPKA, Peter F. STADLER

COMPUTING THE CLUJ INDEX OF THE FIRST TYPE DENDRIMER NANOSTAR

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The Cluj index ($IE(M) = (\frac{1}{2})\sum_i \sum_j [M]_{ij}[A]_{ij}$) is related to the Cluj matrices (**M** =CJD, CJΔ, CFD, CFΔ) but in all graphs: IE(CJD) = IE(CFD); IE(CJΔ) = IE(CFΔ). Thus, to compute the Cluj index is sufficient that only IE(CJD) and IE(CJΔ) are computed. In this paper we compute IE(CJD) and IE(CJΔ) for the first type dendrimer nanostar.

Keywords: Cluj index, Cluj matrix, dendrimer nanostar, molecular graph

CHEMISTRY EXPERIMENTS REPORTS SUBMISSION AUTOMATION

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Automation is becoming indispensable day by day in every field. It may be a business process, or any scientific documents workflow like Academic Project Reports Submission. In this paper, an application of a customizable workflow automation engine in the project report submission in a chemistry lab is introduced. The automation allows students to submit experiments data reports and the manually calculated results to their instructors online. The system facilitates the instructor by automatically calculating the results from the data submitted by the student. Comparing the results from the system and the results manually calculated by the student helps decide the instructor to approve or disapprove the results. Moreover, the Chairman of the dept is provided with a managerial view of all the report submission activities being performed in the dept with their current status. The instructor can also forward any complaint regarding student not submitting report to the registrar for issuing warning.

The advance features of the workflow automation engine include Automatic Sending of email reminders to complete tasks after certain administrator–defined interval, Action Tracking, Processing of Parallel and Sequential Tasks, Easy Concealment of certain role names from others, Easy Method to provide Instructions on each webpage, *etc*.

CALCULATION OF ACTIVATION ENERGY OF KBr:Eu SINGLE CRYSTAL

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Samples, dimensions of about 4x4x3 mm^3, were cutted from a KBr:Eu single crystal block given to us by Library of the Fundamental Research, and grown.

We calculated for them the trapping parameters associated with localized energy levels, namely the activation energy and the frequency.

The TL glows peaks were analyzed by the total curve–fitting method in order to obtain the activation energy, pre–exponential factor and kinetic order.

Two methods, of Lushchik and Halperin, were used to calculate the activation energies. By using these two methods the activation energies for first and second order are introduced and checked.

Simultaneous measurements of the thermoluminescence and thermally stimulated exoelectron emission from this sample were carried out using different post–irradiation annealing temperatures.

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MULTISCALE MODELING OF LOOPS IN PROTEINS: BEYOND CLASSICAL COMPARATIVE MODELING

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Background

Template–target sequence alignment and loop modeling are key components of protein comparative modeling. Short loops can be very accurately predicted using structural fragments from other, not necessary homologous proteins. For longer loops multiscale approaches based on coarse–grained de novo modeling techniques should be more effective.

Results

For representative set of protein structures of various structural classes test predictions of loop regions have been performed using a golden standard of comparative modeling, MODELLER and a coarse–grained de novo modeling tool CABS. Loops of various lengths, from 4 to 25 residues were modeled assuming an ideal target–template alignment of the remaining portions of protein. It has been shown that the classical modeling with MODELLER is usually better in the cases of short loops, while CABS modeling followed by all atom reconstruction is more effective for longer loops. Taking into consideration the above complementary results, a hybrid hierarchical modeling pipeline is proposed, where the models from CABS are used as templates for MODELLER based modeling. On average, the resulting molecular models were significantly better than the models from individual methods. Even for relatively large loops, ranging from 16 to 25 residues, the structures obtained by means of multiscale modeling are usually qualitatively correct, although in the range of residue size resolution.

Conclusions

Even very long missing fragments in protein structures could be effectively modeled using mesoscopic modeling tool CABS. Resolution of such models is usually on the level 2–6 Å, which could be sufficient for guiding protein engineering. Further improvement of the modeling accuracy could be achieved by combination of different methods.

DYNAMIC MONTE CARLO SIMULATION OF URBAN PHOTOCHEMICAL SMOG

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Red–orange NO_2 absorbs sunlight and produces ozone. The second key to urban ozone production is the presence of volatile organic compounds (VOCs) and carbon monoxide. It is the synergistic effect of NO_x, CO, and volatile hydrocarbons that produces photochemical smog. In this study, we use dynamic Monte Carlo Simulation method to understand and assess the process at molecular level. With variable time and distance from source of emissions, concentration profiles are generated. Our model can predict the distributions of concentration at various locations as well as for various daytime from sunrise to sun set. Temperature is a key variable during these simulations. Moreover, number of sources, stationary or moving source, wind velocity and direction, area of emission, height of emission, continuous or puff emission and many other parameters can also be studied with our model. Although it takes more than thousands of runs to get the results but predictions show potential to put up with the model. Figure 1a shows that molecules of smog are increasing with time. At different locations, the linearity is same but comparison with each other shows back ward reactions are occurring for higher concentrations. Further detailed study for this reaction system will be done in this paper.

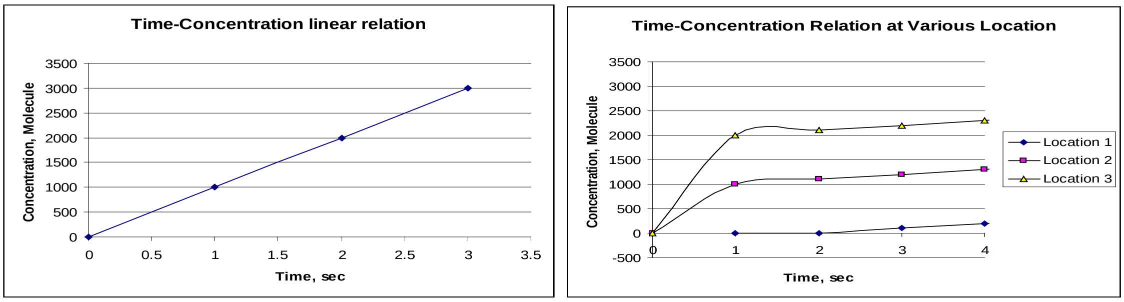

Figure 1. NO_x concentration time relationship (Left) linear for one location (Right) linear but showing some backward reaction at different locations, for photochemical smog.

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THE CUT METHOD AND SOME OF ITS APPLICATIONS IN CHEMICAL GRAPH THEORY

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A general description of the cut method will be presented and an overview of its applications in chemical graph theory given. Applications include the Wiener index, the Szeged index, the hyper–Wiener index, the PI index, the weighted Wiener index, Wiener–type indices, and classes of chemical graphs such as trees, benzenoid graphs and phenylenes. Algorithmic issues will also be briefly mentioned.

ON USING GRAPHICAL INVARIANTS AS AMINO ACID DESCRIPTORS

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Graphical invariants such as the domination number of a graph have been highly studied in graph theory. Applications of the domination number of a graph can be found in fields such as the design and analysis of communication networks and fault–tolerant computing. In this work we model the side chains of the twenty most prevalent amino acids by simple graphs. We select a total of seven highly studied mathematical graphical invariants; the domination number and the upper domination number as well as the diameter, radius, circumference and the average degree. We also define and calculate the maximum peripheral weight invariant. The results verify that these graphical invariants may be used as valid measures of similarity/dissimilarity of amino acids.

DEVEPOLEMENT OF THE METHOD FOR PREDICTING METABOLITES BY USING CHEMOINFORMATICS METHODS

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Purpose of the study

In drug discovery process, it is important to know pharmacological properties of metabolites from the viewpoint of side effects prevention and other issues. Thus, identification of metabolites is a very important task. If metabolites of a drug candidate turn out to have toxicity by clinical trial, cost will have been wasted. In order to avoid such problems, a technique for predicting metabolites beforehand has been hoped. In this study, we have developed a method for predicting metabolites by using chemoinformatics methods.

Methods

Cytochrome P450 (CYP450) is the group of enzymes that is deeply related to drug metabolizing. If we can know isoform specificity and regioselectivity, we can predict metabolites of each drug candidates.

Isoform specificity means: *Whether a drug candidate is metabolized or not by each CYP450?*

Regioselectivity means: *Which site of the molecule is a site of metabolism?*

Therefore, we constructed two models, which are used to predict isoform specificity and regioselectivity, respectively. In order to build an isoform specificity model, we used Random Forest (RF) as a learning method.[1] RF is one of the promising machine learning methods and have high predictive power. We used one of the most frequently used descriptors, Dragon,[2] as explanatory variables. And in order to build a regioselectivity model, we also used RF as a learning method and three kinds of original descriptors as explanatory variables. The descriptors are activation energy of hydrogen abstraction by CYP3A4,[3] solvent accessible surface area, and hydrogen bond donor or acceptor in a molecule. Hydrogen bond donor or acceptor in a molecule represents pharmacophore point of a molecule. Substrates and non–substrates of CYP3A4, which is the main drug–metabolizing enzyme, were used for model building.

Result

As for the isoform specificity model, the accuracy is over 70%. As for the regioselectivity model, the model is succeeded to predict sites of metabolism precisely about 80% of substrates.

Conclusion and Reference

In this study, we have built two models by using chemoinformatics methods in order to predict metabolites of drug candidates. Accuracy of both models are high, and therefore, we could identify metabolites quickly and precisely by using this method.

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ON SUM–CONNECTIVITY INDICES

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COORDINATION SEQUENCES FOR SEMI–REGULAR TILINGS OF THE PLANE

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The coordination sequence (CS) is a number sequence, introduced in order to investigate the topological identity of frameworks and of atomic positions within a framework. The *k*–th term of a CS is the number of atoms in *shell k* that are bonded to atoms in *shell k*–1. Shell zero consists of a single atom, and the number of atoms in the first shell is the conventional coordination number. In graph theory, the CS is also known as the growth of a graph since the *k*–h term represents the number of vertices at distance *k* from some initial vertex.

A tiling of the Euclidian plane is made up of a family of polygons, such that their union is the entire plane and the interiors of the tiles are pairwise disjoint. Furthermore, in a semi–regular tiling each tile is a regular polygon and all vertices are of the same type, i.e. the polygons about each vertex in a cyclic order are the same.

The generating functions that reveal the CSs of all possible semi–regular tilings are presented as well as the method for their calculation.

OLIVE OIL: TECHNOLOGY, CHEMISTRY AND HEALTH

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Olive oil is key component of the traditional Mediterranean diet, which is believed to be associated with a relatively long life in a good health. Olive oil as important and valuable commodity is often adulterated.

In this presentation it will be discussed:

- way of production with respect to olive oil quality,
- chemistry of olive oil, its composition, possible ways and detection of adulteration,
- influence of olive oil components on health.

COMPUTING EDGE SZEGED INDEX OF NANOCONES

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The edge Szeged index is a new molecular structure descriptor equal to the sum of products $m_u(e)m_v(e)$ over all edges $e = uv$ of a molecular graph G, where $m_u(e)$ is the number of edges whose distance to vertex u is smaller than the distance to vertex v, and $m_v(e)$ is defined analogously. In this paper, the edge Szeged index of a general carbon nanocone is computed for the first time.

Keywords: carbon nanocone, edge Szeged index

TOTAL DOMINATION ON LINEAR AND DOUBLE HEXAGONAL CHAINS

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For any graph G by $V(G)$ and $E(G)$ we denote the vertex–set and the edge–set of G, respectively. For graph G subset D of the vertex–set of G is called a dominating set if every vertex $v \in V\backslash D$ is adjacent to at least one vertex in D. The domination number $\gamma(G)$ is the cardinality of the smallest dominating set.

Set D is a total dominating set if every vertex $v \in V$ is adjacent to at least one vertex of D. The total domination number $\gamma_t(G)$ is the cardinality of the smallest total dominating set.

Chemical stuctures are conveniently represented by graphs, where atoms correspond to vertices and chemical bounds correspond to edges.

With $B(h)$ we denote the linear hexagonal chain, also known as linear benzenoid chain, with h hexagons, while with $B(2h)$ we denote the double hexagonal chain with $2h$ hexagons.

In this paper we examine total dominations on linear and double hexagonal chains and determine total domination numbers for such graphs.

THE COLOR RECONSTRUCTIONS OF IMAGES BY GRAPH THEORY

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Fuzzy sets defined on the Hue, Saturation and Value components of the HSV color space, provide a fuzzy logic model that aims to follow the human intuition of color classification.

In this paper we describe a human perception based approach to pixel color segmentation which is applied in color reconstruction by numerical method associated with graph–theoretic image processing algorithm, typically in grayscale. The proposed model introduces an improvement over some other basic color classification techniques which are considered more challenging to color segmentation methods. In color vision systems require a first step of classifying pixels in a given image into a discrete set of color classes.

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COMPUTATIONAL MODEL STUDY ON THE AVALANCHES DYNAMICS

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Snow is assumed to be represented by semi-solid and the governing equations have been studied from the concept of continuum approach. The avalanche release of snow has been modeled.[1-3]
In this paper, by using appropriate initial and boundary conditions, the dynamical equations[2] have been solved for three following different zones:

(i) starting zone,
(ii) uniform zone, and
(iii) run out zone, furthermore velocity has been computed for the above zones.

Effect of the density (ρ), Eddy viscosity (η), Slope angle (θ), Slab depth (R and H) on the flow parameters have been observed. Furthermore, for computing the non linear differential equations, numerical methods have been employed. The out puts have been compared with results given in Ref. 1. One of the most interesting and fundamental innovation in the present studies is getting initial condition for the computation of velocity either by numerical or by analytical approach. The information of the velocity has been obtained through the concept of fracture mechanics applicable to snow.[4]

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DEVELOPMENT OF A NEW PSEUDOPOTENTIAL FOR ELECTRON–METHANOL SYSTEM

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Solvated electron has long been investigated because of its importance in fundamental chemistry and several biological processes. With the rapid advance of experimental techniques the negatively charged solvent clusters have once again become in the center of scientific interest recently. The interest is mainly motivated by the fact that cluster anions can serve as a bridge to understand the transition from gaseous species to the bulk solvated electron.

Despite the finite size and the anticipated relative simplicity of cluster anions compared to bulk condensed phases, up to now there is still no consensus on the most basic structural properties of water cluster anions.[1] A straightforward approach to solve the problematic issues is to extend the investigations to other polar solvents.

In this work we decided to develop a new pseudopotential for electron–methanol system which is the first step for the theoretical investigation of the properties of methanol anion clusters. Since the full many–electron treatment of such system is still out of reach, approximative techniques have to be used. A commonly used approach is the mixed quantum–classical molecular dynamics (QCMD) where the solute is treated by quantum mechanically, while the surrounding solvent molecules are described by classical potentials. In the case of solvated electron systems the interaction between the quantum object (the excess electron) and the solvent molecules can be taken account using electron–solvent pseudopotentials. The new potential has the form based on the parametrization by Turi and Borgis (TB) for the electron–water system.[2] The main point of our new pseudopotential set is the transferability: for the hydroxyl oxygen and hydrogen we used the same parameters which were developed for the water and the parameters of the carbon and methyl hydrogens were optimized reproducing the experimental optical absorption spectra of a large methanol cluster of 500 molecules. The development of pseudopotential, the optical absorption spectra and other properties of the cluster are presented.

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THE WIENER AND DETOUR INDICES OF AN INFINITE CLASS OF DENDRIMER NANOSTARS

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Let G be a molecular graph. The Wiener and detour indices of *G* are defined as the sum of the lengths of all shortest and longest paths between vertices of *G,* respectively. In this paper at first all parts of nanostar dendrimers are classified and then exact formulae for the Wiener and detour indices of them are given.

Keywords: detour index, molecular graph, nanostar dendrimer, Wiener index

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IN THE EYE OF THE BEHOLDER: INHOMOGENEOUS DISTRIBUTION OF HIGH–RESOLUTION SHAPES WITHIN THE RANDOM–WALK ENSEMBLE

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The concept of high–resolution shapes of a polymer chain plays a central role in polymer science, structural biology, bioinformatics and biopolymer dynamics. However, although the idea of shape is intuitively very useful, there is no unambiguous mathematical definition for this concept. In the present work, the distributions of high–resolution shapes within the ideal random–walk ensembles with N = 3..6 beads (or up to N = 9 for some properties) are investigated using a systematic (grid–based) approach, based on a simple working definition of shapes relying on root–mean–square atomic positional deviation as a metric (*i.e.*, to define the distance between pairs of structures) and a single cut–off criterion for the shape assignment. Although the random–walk ensemble appears to represent the paramount of homogeneity and randomness, this analysis reveals that the distribution of shapes within this ensemble, *i.e.*, in the total absence of interatomic interactions characteristic of a specific polymer (*i.e.*, beyond the generic connectivity constraint), is significantly inhomogeneous. In particular, a specific (densest) shape occurs with a local probability that is 1.28, 1.79, 2.94 and 10.05 times (N = 3..6) higher than the corresponding average over all possible shapes (these results can tentatively be extrapolated to a factor as large as about 1028 for N = 100). The qualitative results of this analysis lead to a few rather counter–intuitive suggestions, namely that *e.g.*:

(*i*) a fold classification analysis applied to the random–walk ensemble would lead to the identification of random–walk *folds*;
(ii) a clustering analysis applied to the random–walk ensemble would also lead to the identification random–walk *states* and associated relative free energies;
(*iii*) a random–walk ensemble of polymer chains could lead to well–defined diffraction patterns in hypothetical fiber or crystal diffraction experiments.

MOLECULAR ORBITAL CALCULATION BEYOND ADIABATIC APPROXIMATION: MULTI–COMPONENT MOLECULAR ORBITAL METHOD

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The problem imposed on quantum chemistry is to clarify chemical concepts or chemical phenomena under the quantum mechanical principle. For example, the nuclear quantum effects, such as zero point energy, nuclear tunneling, and vibrational excitations, are interesting subjects in chemistry, as well as in physics and in other interdisciplinary fields. Also, many phenomena induced by the H/D isotope effect are observed experimentally, such as the red shift of the vibrational frequency, the change in the chemical reaction rate, the Ubbelohde effect, and a drastic change in the phase transition temperature of hydrogen–bonded dielectric materials. Moreover, biological reactions involving hydrogen often can be dissected using deuterium substitution. It is, however, sometimes difficult to theoretically describe these nuclear quantum effects within only the Born–Oppenheimer approximation.

For molecular systems, to theoretically evaluate the nuclear quantum nature accounting for the H/D isotope effect, we have proposed the multi–component molecular orbital (MC_MO) method to determine both nuclear and electronic wave functions simultaneously. We have already found that the MC_MO method has great success in analyses of the geometrical isotope effect (GIE) in C–H…O hydrogen bonds *etc*. The MC_MO method is also a powerful tool for analyzing the hydrogen (proton) transfer reaction mechanism in terms of the kinetic isotope effect (KIE). Recently, we have developed a fragment MO (FMO) –MC_MO method to analyze H/D isotope effect for large molecules. We would like to explain the methodology and applications of MC_MO method.

INVESTIGATION OF THE STRUCTURE, ENERGY AND VIBRATIONAL FREQUENCY IN SOME INORGANIC AND ORGANIC COMPOUNDS INCLUDING B AND N ATOMS BY *ab Initio* METHODS

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Several molecular properties such as energies, dipole moments, total charge on boron atoms, HOMO and LUMO orbital levels, gap energies and N–B and B–H harmonic frequencies and effects of boron atom on N-H frequencies are investigated on 10 numbers of inorganic and 20 numbers of organic molecules with two different *ab initio* methods, RHF and B3LYP with 6–31G** basis set, and semi empirical method, AM1.

In inorganic group, the energy decreases with –NH2 substitution, when the number of nitrogen atoms increases. The dipole moment increases with first substituent but gradually decreases when the number of nitrogen atoms increases. Total atomic charge on boron atom increases with increasing the number of nitrogen atoms. But the gap energy has a decreasing trend.

In the cyclic molecules, there is a same charge on the boron atoms because of the same conditions, but in the chain molecules the boron atom attached to one nitrogen atom has a one half charge that of the boron atom attached to two nitrogen atoms. For B–H, the bending frequencies in the ring and chain molecules appear in 300- 400 cm^{-1} and 1000 cm^{-1}, respectively.

In the organic group, the energies decrease with increasing the number of substitute. Total positive atomic charge on born atom increases because of electron accepting character of –CN substitute. The dipole moment has a decreasing manner with increasing molecular symmetry. The gap energy has a decrease trend too. Also the saturated effect and breaking bond in the ring molecules has been considered.

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DETERMINATION OF OLIVE OIL ADULTERATION WITH CHEAPER VEGETABLE OILS USING INFRARED AND FLUORESCENCE SPECTROSCOPY TECHNIQUES COUPLED WITH GENETIC MULTIVARIATE CALIBRATION

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Determination of authenticity of extra virgin olive oils has been an important issue in recent years due to the increasing public concerns about possible adulterations with relatively cheap vegetable oils such as sunflower oil and corn oil. This study was focused on the application of molecular spectroscopy (Near infrared, Mid infrared and Fluorescence) in conjunction with multivariate calibration to determine adulteration of olive oils. Molecular spectroscopic techniques provide a fast and usually solvent free determination of multicomponent mixtures especially when the component concentrations are relatively large. Adulteration of olive oils with cheaper substitutes generally results with large quantities of adulterants, and thus the above mentioned spectroscopic methods could be effective screening tolls. Spectroscopic measurements were made on pure olive oil and olive oil adulterated with varying concentrations of different vegetable oils in a sets of 50 ternary mixtures. Multivariate calibration models were generated using genetic inverse least squares (GILS) method and used to predict the concentration of adulterants along with the concentration of olive oil in the samples. The GILS method is a genetic algorithm based multivariate calibration method which selects the most appropriate wavelengths over an entire spectral region for each component in the mixtures. Over all, standard error of predictions ranged between 0.51% and 1.27 % (w/w %) for the mixtures of olive oil and other different vegetable oils. The results indicated that selected molecular spectroscopic techniques coupled with multivariate calibration can be used to determine adulteration of olive oil with other vegetable oils without any sample preparation.

Keywords: fluorescence spectroscopy, genetic algorithms, infrared spectroscopy, multivariate calibration, olive oil adulteration

CONFORMATIONAL ANALYSIS OF CYCLIC MOLECULES: GENERAL APPROACHES BASED OF PUCKERING PARAMETERS

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The conformational analysis of cyclic molecules is an important field of stereochemistry. A number of approaches based on the so called puckering parameters had been introduced in literature for the quantitative description of ring conformations. The shape of N–membered ring is quantitatively described by only $N - 3$ puckering parameters (amplitudes and phase angles). We had suggested the system of puckering parameters based on the angular characteristics of rings which are applicable to cyclic molecules containing various hetero atoms. This approach has been successfully applied to analyze in detail the conformational space of 4– ÷ 10–membered rings in monocyclic and polycyclic molecules. In order to further decrease the number of independent parameters for macrocyclic molecules the pseudocycle puckering approach has been developed and used to characterize the spatial arrangements of heteroatoms in 15–crown–5 and 18–crown–6 complexes by only two and three puckering parameters, respectively.

The puckering parameters can serve as convenient coordinates for the consideration of any conformational changes in cyclic molecules.

THE IMPACT OF ALPHA-MELANOCYTE-STIMULATING HORMONE ON THE CORNEAL RE-EPITHELIALIZATION IN RATS

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Alpha–melanocyte–stimulating hormone (α–MSH) is one of the initial fragments of the molecule ACTH. Additional to its role in skin–darkening, α–MSH also possesses a strong immuno–modulating, anti–inflammatory, antipyretic and antimicrobial properties. Its cytoprotective properties are also known, realised through inhibition of pro–inflammatory cytokines and the impact, inhibition of NO and neopterin synthesis by monocytes, inhibition of neutrophil migration and synthesis of prostaglandin as well as the increased production of IL–10. Alpha–MSH has also been found in some eye structures including the cornea. However, its role in corneal re–epithelialization has not been sufficiently examined.

In this study we intended to analyse the impact of α–MSH on the corneal re–epithelialization, reduction of eye irritation caused by epithelium erosion and the possibility of blocking its impact with the complementary peptides.

Test animals were assigned into nine (9) groups which were treated as follows: the control group was treated by physiological solution, 5 groups by α–MSH drops in concentration ranging from saturation to inefficiency, 2 groups were treated by α–MSH drops in ED_{50} and $ED_{50}/10$ doses together with the equimolar dose of complementary peptide, and one group of healthy animals to which the most effective α–MSH dose was applied. Drops were applied immediately after eroding, after 2, 8 and 16 hours. The photographs were taken every 0, 2, 8 16 and 24 hours. After test completion the histological analysis of cornea was made, the photographs digitally evaluated, and the erosion extent defined.

Alpha–MSH has caused a faster rate of epithelialization in concentrations of 1 mg/100 ml, 1 mg/1000 ml and 1 mg/10000 ml 16 hours after debridement and the latter two concentrations 24 hours after debridement, respectively. By antisense peptides the possibility of impact blocking has been established. In several concentrations a significant decrease of eye stimulus was established. Histological slices have shown a decreased number of neutrophils in corneas treated by α–MSH in contrast to the control group.

In view of the mentioned results it would be beneficiary to undertake further study of the α–MSH role in the re–epithelialization as a potentially useful peptide to be used in the human medicine.

ENUMERATION OF TOROIDAL POLYHEXES – TOWARDS A CLOSED FORM SOLUTION*

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A closed form solution to the enumeration problem of toroidal polyhexes is presented. It is shown that the question under what conditions toroidal polyhexes are considered the same (or isomorphic) may be answered in more than one legitimate way. This explains why some numbers computed in the past do not agree. This talk presents the current sate of the work in progress that resulted from a fruitful collaboration with E.C. Kirby, R. Mallion and P. Pollak.

Keywords: divisor function, enumeration, toroidal polyhex

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[*] **MSC (2000) 05 C 10, 57 M 15, 05 C 30**

THE ALTERATION OF LIPOPROTEINS AND LIPID CONCENTRATIONS FOLLOWING AEROBIC EXERCISE ON MALE STUDENTS

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The purpose of this research is to study the effects of aerobic exercise on blood serum lipids. For this purpose, 13 male students were tested twice a week during eight weeks. The concentrations of cholesterol, triglyceride, low density lipoproteins (LDL) and high density lipoproteins (HDL) in blood sera were determined before and after exercise. In the first four sessions the running distance was set on 140 – 150 heart beats. In the last four sessions the running distance increased to 3200 meters and intensity of heart rate reached 180 beats. The results obtained for the concentrations of serum lipids (Table 1) were analyzed using SPSS statistic software.

Table 1. Serum lipid concentrations determined before and after aerobic exercise

SERUM LIPIDS	CONCENTRATIONS (mg/dl)		*t*	P
	BEFORE TRAINING M.V.±S.D*	AFTER TRAINING M.V.±S.D*		
Cholesterol	176.77±32.60	169.77±37.26	1.511	0.75
Triglyceride	127.15±37.28	102.77±28.00	2.499	0.028
HDL	45.23±6.65	45.38±8.58	0.08	0.938
LDL	106.15±28.94	97.69±28.59	2.91	0.013

*M.V.±S.D = mean value±standard deviation

The exercise had not influence on HDL concentration. The decrease of cholesterol concentration before and after exercise was not significant statistically (P = 0.75). A significant decrease of triglyceride concentration (P = 0.028) and LDL concentration (P = 0.013) before and after exercise were found. These results showed that continuous incremental aerobic running during eight weeks can be effective on decreasing of the concentrations of blood serum lipids and lipid metabolism.

Keywords: aerobic exercise, serum lipid concentration

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EFFECT OF STRESS ON BLOOD PRESSURE AND HEART RATE OF HIGH SCHOOL GIRLS

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The aim of this study was to monitor the changes of systolic blood pressure, diastolic blood pressure, and heart rate the in the high school girls during the period of the examination, particularly during the physics exam. For this purpose, 58 students were randomly selected (age: 16.58 ± 0.56 years old, height: 157.89 ± 6.64 cm, weight: 53.72 ± 7.3 kg, and body mass index – BMI: 21.08 ± 2.96). In the first phase, prior to the examination, systolic and diastolic blood pressure and heart rate relaxation state were measured and recorded. The second phase of the study was carried out after 28 days in the period of examinations and the same parameters were measured 15 minutes prior to the physics exam. The results, analysed using the one sample *t*–test, proved that there is a significant difference between the average systolic and diastolic blood pressure determined in the first and the second phases ($P = 0.002$). Moreover, the significant differences between the individual average values of the heart rates measured in the first and second phases were obtained. The results of this study proved that the high school physics examination might cause significant changes in the blood pressure and the heart rate of the high–school students.

Keywords: blood pressure, heart rate, stress

NATURAL DISTANCE MATRIX

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ESTIMATION OF STABILITY CONSTANTS OF COORDINATION COMPOUNDS USING CONNECTIVITY INDEX $^3\chi^v$

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In contrast to QSPR of organic compounds, where variety of topological indices are checked to obtain as good as possible agreement with experimental data, in the case of coordination compounds one of the topological indices was chosen to be calculated from variety of graphs (*i.e.*, constitutional formulas) connected with the studied system. Thus, for the estimation of stability constants of copper(II) and nickel(II) chelates with diaminoethanes and copper(II) chelates with amino acids and their *N*–alkylated derivatives we used graphs of the ligands (L), graphs of *mono*– (ML) and *bis*–complexes (ML_2), and also graphs of di*aqua*–complexes (ML^{aq} or ML_2^{aq}). Moreover, we introduced «dummy» bonds between side chains of ligands and central atom to model non–bonded interactions in molecule (graphs ML^{cor} and ML_2^{cor}). In all our calculations we used exclusively connectivity index of the 3rd order ($^3\chi^v$), that proved best.

Our results clearly show that more realistic graph leads to more successful estimation of stability constants. We also compared our estimates for copper(II) chelates with alanine and its *N*–alkylated derivatives with experimental constants obtained by two electrochemical methods, and found our theoretical approach suitable for discussion of experimental results and methods.

APPLICATION SELF–CONSISTENT ORNSTEIN–ZERNIKE AND MEAN SPHERICAL APPROXIMATION FOR STUDY BINARY YUKAWA SYMMETRIC FLUID MIXTURE

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In this study we have used Self–Consistent Ornstein–Zernike (SCOZA) Approximation and Mean Spherical Approximation (MSA). By comparison of these methods, we can calculate Gibbs free energy, thermodynamic behaviour and phase diagrams. The SCOZA is an advanced method achieved by enforcing thermodynamic self–consistent between the compressibility and the energy way. Each of phase diagrams is characterized by a specific critical behaviour. The phase diagrams are discussed by solving the existence equations, *i.e.*, equal chemical potentials and equal pressure of the coexisting phases at a system temperature. MSA and SCOZA were applied on the fluid for different dipolar moment and the properties of fluid and internal energy of fluids were discussed. To study the limits of thermodynamic stability becomes for a fluid mixture a noticeable more complex problem than in the one component case, for a composition, density, pressure and temperature the requirements for both physical and chemical stability can be fulfilled. It was found that the MSA solution is reasonable only at lower dipole moments, while the perturbation theory gives good results at low and high values of dipole moment.

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HOST/GUEST NANOCOMPOSITE MATERIALS: THERMODYNAMIC THEORETICAL CALCULATION, SYNTHESIS AND LIQUID PHASE OXIDATION OF OXIDATION OF CYCLOHEXENE WITH MOLECULAR OXYGEN

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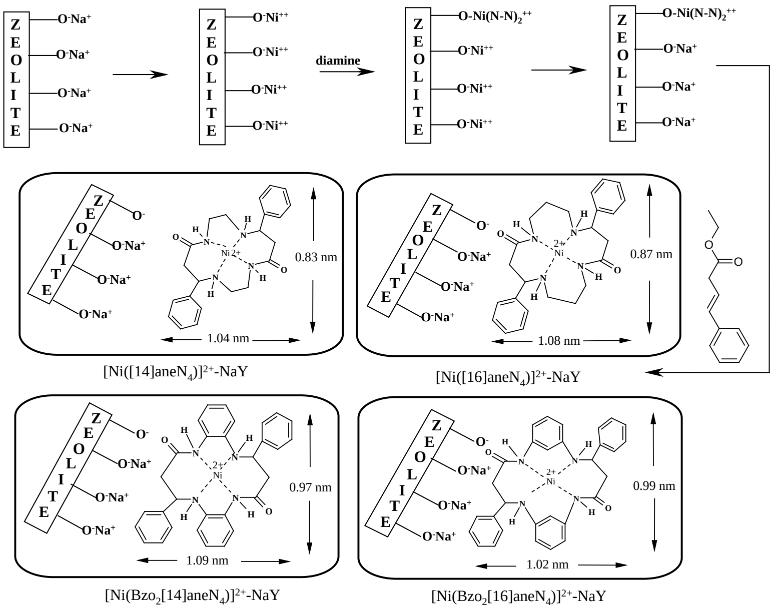
Thermodynamic properties of 14– and 16–membered tetraaza dioxa diphenyl nickel(II) complexes by using of Computational methods are theoretical calculated and then nanocavity microreactor containing 14– and 16–membered tetraaza dioxa diphenyl nickel(II) complexes have been encapsulated in the nanopores of zeolite–Y by a two–step process in the liquid phase:

(i) adsorption of [bis(diamine)nickel(II)] (diamine = 1,2-diaminoethane, 1,3–diaminopropane, 1,2–diaminobenzene, 1,3–diaminobenzene); $[Ni(N\text{-}N)_2]^{2+}$-NaY; in the nanopores of the zeolite–Y, and

(ii) in situ condensation of the nickel(II) precursor complex with ethylcinnamate.

The new host–guest nanocomposite materials (HGNM) were characterized by several techniques: chemical analysis and spectroscopic methods (FT–IR, UV/Vis, XRD, and DRS) and BET technique. These complexes were used for oxidation of cyclohexene with molecular oxygen.



Scheme 2.

Keywords: macrocycle, theoretical calculation, nanocomposite materials, nanopores, nickel(II), oxidation of cyclohexene, tetraaza dioxa

AN OVERVIEW TO THE WORLD OF COMPUTATIONAL CHEMISTRY

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The term theoretical chemistry may be defined as the mathematical description of chemistry. The term computational chemistry is usually used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer. Note that the words exact and perfect do not appear in these definitions. Very few aspects of chemistry can be computed exactly, but almost every aspect of chemistry has been described in a qualitative or approximate quantitative computational scheme. The biggest mistake that computational chemists can make is to assume that any computed number is exact. However, just as not all spectra are perfectly resolved, often a qualitative or approximate computation can give useful insight into chemistry if you understand what it tells you and what it doesn't. The most famous methods of computational chemistry are as following:

- *ab Initio*,
- Semiempirical,
- Modelling the Solid State,
- Molecular Mechanics,
- Molecular Dynamics,
- Statistical Mechanics,
- Thermodynamics,
- Structure–Property Relationships,
- Symbolic Calculations,
- Artificial Intelligence.

In this presentation all methods mentioned above are discussed.

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MOLECULAR INVOLUTORY FORMS FOR COORDINATION AND NON-COORDINATION COMPOUNDS

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Empirical chemistry recognizes at least two stages of molecular constitution. Forms of molecules can equivalently be expressed in terms of involutory injections. Basic mathematical features of them are supposed to be of empirical relevance. The parity and the number of involutory injections have been established for a general case of coordination and non–coordination compounds treated jointly. The approach is tested and discussed in the context of receiving surplus information on molecular self–assemblage structures. An axiomatic system has been proposed as a tool needed in proving mathematical peculiarities implied by functions underlying molecular symmetries.

USING ORDER AND SIZE FOR BOUNDING EXPRESSIONS OF GRAPH INVARIANTS

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Systems for automatized scientific research can be of great help to scientists at their research. One of such systems is AutoGraphiX – system for automatized scientific research in graph theory. System is based on the Variable neighborhood search (VNS). The basic problem is minimization (maximization) of the function *f*(*G*) which is expression of one or more graph invariants, and to that problem reduce various tasks which the system deals with. The system AutoGraphiX generated conjectures in basic form $\underline{b}(n) \le i_1 \otimes i_2 \le \overline{b}(n)$, where i_1 and i_2 are graph invariants, $\otimes$ one of the four basic operations $+, -, \bullet, /$, $\underline{b}(n)$ and $\overline{b}(n)$ lower und upper bound in number of vertices *n* of the graph. The variant of the basic form, *i.e.*, the form $\underline{b}'(m) \le i_1 \otimes i_2 \le \overline{b}'(m)$ was also considered which differs from the basic form in that the bounds $\underline{b}'(m)$ and $\overline{b}'(m)$ depend on number of edges *m* of the graph. We will show the results of the systematic analisys of the research, and the examples of the most interesting conjectures, proven or refuted.

OUR VIEW ON PROTEIN STRUCTURES IN THE CURRENT, POST–GENOMIC ERA

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The genome projects have significantly extended the scope of investigated proteins. First, transmembrane proteins have been shown to be of much higher proportion among proteins than ever thought, before. Later the existence of partially or fully disordered proteins and their surprisingly high representation in eukaryotic organisms have been detected, as well as their key role in signal transduction and regulation processes. All these new knowledge resulted in a new view on protein structure and on structure–function relationship. Fast development in computational technology in the recent two decades, including the establishment of the World Wide Web, also has great influence on protein science. In my lecture I will talk about some recent results on *traditional* globular proteins as well as on transmembrane and disordered/unstructured ones.

Considering the *traditional* globular proteins, we can learn a lot about their functionally relevant dynamic properties in enzyme action, macromolecular recognition *etc*. *via* computation. As a new result in transmembrane protein topology prediction, I will show how a new database TOPDOM can improve the accuracy of our most popular prediction method, HMMTOP. In the field of disordered proteins the functional role of protein disorder in numerous cases, including the analysis of dUTPase, the substrate preference of transglutaminase and the involvement of the mediator complex in transcriptional regulation will be discussed. Also, some fundamental results that enabled the characterization of interacting regions in disordered proteins will be presented together with the development of a method, called ANCHOR for the prediction of such disordered binding sites.

Finally some new principles of protein structure formation will be discussed.

SEQUENCE ALIGNMENTS ON A META LEVEL: STRUCTURAL PATTERNS AND COMPARATIVE EVIDENCE METHODS IN RNA PHYLOGENY RECONSTRUCTION

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Ribosomal RNA genes are probably the most frequently used source of data in phylogeny reconstruction. They are highly structured, with large parts of the molecules exhibiting very strong conservation of their base pairing patterns. Therefore, it is natural to improve alignment accuracy by incorporating information about secondary structure conservation. However, as a consequence of their highly conserved secondary structures, individual alignment columns can be very strongly correlated. Unless explicitly taken into account, these correlations will distort phylogenetic signals and/or lead to overestimates of tree stability. While Bayesian approaches are amenable to using RNA-specific substitution models that treat conserved base pairs appropriately, so far there has not been a sufficiently accurate and performing tool for computing structure-aware alignments and consensus structures that can deal with the large ribosomal RNA sequences. The `RNAsalsa` approach is designed to fill this gap. Capitalizing on the improved accuracy of pair wise consensus structures and informed by a priori knowledge of group–specific structural constraints, the software provides alignments and consensus structures, as well as individual secondary structure predictions that are of sufficient accuracy for routine phylogenetic analyses based on RNA–specific substitution models. We could demonstrate the power of the approach using various datasets of mitochondrial rRNAs and collections of nuclear 28S rRNAs.

The software package `RNAsalsa` serves as an easy–to–use framework with a focus on concurrent computations of improved RNA structure predictions and alignments of structural RNA sequences. It utilizes prior knowledge about structural patterns, adapted constraint directed thermodynamic folding algorithms, and comparative evidence methods. It automatically and simultaneously generates both highly corrected individual secondary structure predictions within a set of homologous RNA genes and a consensus structure for the whole set, and it takes then sequence and structure information into account as part of the alignment's scoring function; *i.e.*, `RNAsalsa` uses structure information for adjusting and refining the sequence alignment and vice versa.

Phylogeny reconstruction tasks are the main group of applications for `RNAsalsa`; methods can easily be extended to RNA secondary structure, incorporating both the `RNAsalsa` derived (and mostly improved) models for the secondary structure elements of the RNA and also the alignment based on that extended structure information. Thus, it is possible to make the slower evolution of the structural features a reproducible source of information.

The current version of `RNAsalsa` is command line based and available either as source code, or as a pre-compiled executable for various common operating systems. `RNAsalsa` is written in C, all sources and executables as well as a detailed manual may be downloaded from
`http://www.rnasalsa.zfmk.de/`
and from
`http://www.bioinf.uni-leipzig.de/Software/RNAsalsa/`

INVESTIGATION OF LEVEL CROSSING FOR COMPLEX QUANTUM SYSTEMS

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Complex systems, such as molecular, atomic, nuclear ones are characterized by some degrees of freedom, separation of which in strongly interacting systems, as a rule, are not valid. We investigate the role played by level crossing for collective motion in the presence of *fast* dynamics of separate particles in the system within the adiabatic representation method, which is one of the most useful methods in the treatment of the quantum dynamical systems with some degrees of freedom. The method permits one to construct a wide class of potentials and corresponding solutions of the parametric equation in a closed analytical form and, after that, to calculate the matrix elements of the exchange interaction. It was shown that in the case of the parametric problem on the entire axis the induced scalar and vector potentials and the basis functions are not singular at the degeneracy points of the two states, while in the parametric problem on the half–axis, the potential, together with its eigenfunctions and matrix elements of the exchange interaction, are singular at these points. In particular, we have found that in the parametric problem on the entire axis for a special choice of the normalization functions, the potential is transparent and symmetric and the exchange interaction between the bound states for two–level systems are equal to zero for all values of the parametric variables, even at the point of the degeneracy.

INTRINSIC GEOMETRY OF CYCLIC HEPTAGONS AND OCTAGONS

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Finding formulas for the area or circumradius of polygons inscribed in a circle in terms of side lengths is a classical subject. For the area of a triangle we have famous Heron formula and for cyclic quadrilaterals we have Brahmagupta's formula. A decade ago D.P. Robbins found a minimal equations satisfied by the area of cyclic pentagons and hexagons by a method of undetermined coefficients and he wrote the result in a nice compact form.[4] The method he used could hardly be used for heptagons due to computational complexity of the approach. In another approach with two collaborators[2] a concise heptagon/octagon area formula was obtained recently (not longer after D.P. Robbins premature death). This approach uses covariants of binary quintics. It is not clear if this approach could be effectively used for cyclic polygons with nine or more sides. A nice survey on this and other Robbins conjectures is written by I. Pak.[4]

In this talk we shall present an intrinsic proof of the Robbins formula for the area (circumradius and area times circumradius) of cyclic hexagon based on an intricate direct elimination of diagonals (the case of pentagon was treated in Ref. 5) and using a new algorithm from Ref. 6. In the early stage we used computations with MAPLE (which sometimes lasted several days, nowdays several hours!). Based on our new intermediate Brahmagupta formula we get simpler systems of equations for the area and area times circumradius of cyclic heptagons and cyclic octagons.Also computations of all diagonals will be discussed.[10] It seems remarkable that our approach, with a help of Groebner basis technics leads to minimal equations ,what is not the case with iterated resultants approach.

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MONITORING DYNAMICS OF CROATIAN OLIVE FIELDS AND VINEYARDS USING REMOTE SENSING APPLICATIONS

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The European Economic Community since 1975 has placed regulations concerning the management of the olive oil market sector. Counting olive trees is crucial for the European Union olive production subsidies. This kind of statistical survey is important for the implementation of registers of olive fields and vineyards in Croatia which are the basis for the crop management within the frame of the Common Agricultural policy of the European Union. Up until now the accounting of olive trees in Croatia is generally based on data submitted by the plantation owners.

This project aims to provide the assessment of number of olive trees in the Marina region in Dalmatia. Using high spatial resolution multispectral imagery (QuickBird) we will be able to identify and individually position olive trees within the area. In accordance with the European Union, we will use remote sensing with Very High Resolution (VHR) satellite images (QuickBird) to identify and individually position olive trees within the area. QuickBird images (Digital Globe) in Panchro and Pansharp mode (0.6 m pixel resolution) will be acquired over the Marina region. The Joint Research Centre (JRC) designed, an automatic counting tool named OLICOUNT will be used for counting olive trees. OLICOUNT operates with four parameters: grey value threshold, tree diameter, crown shape, and crown compactness.

Remote sensing is a valuable tool for agricultural statistics. If this remote sensing technology is adapted by Croatian scientists, future statistical survey of crops and fruit trees in Croatia will be cost-efficient and more effective. This project will enhance future counting and monitoring of olive fields and vineyards across the whole country using remote sensing technology. Quality and quantity of both wine and olive products will be regulated in the coming years when Croatia is expected to become a member of the European Union and when the export of these products will be an important part of the Croatian economy.

Our intention is also to introduce remote sensing as a technology that can be applied to other fields as well. The results generated at this project stage will be used in the subsequent phases, where we will explore the quality of the olive fields and vineyards using hyperspectral remote sensing (*Hyperspectral Remote Sensing Applications in Monitoring Dynamics of Croatian Vineyards and Olive Fields*). Biochemical and biophysical parameters of fruit crops are crucial indicators of their health, fruit quality and yield. Biochemical constituents are, in particular, important indicators of chlorosis due to plant stress and nutritional deficiencies. A number of studies have indicated the feasibility of chlorosis detection through chlorophyll content estimation using either spectroscopy or optical indices proposed to relate remote sensing data to crop status.

PHOTOCHEMICAL ELECTROCYCLIZATION OF THE NOVEL STYRYL–SUBSTITUTED FURO–BENZOBICYCLO[3.2.1]OCTADIENE DERIVATIVES

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New strategy for the synthesis of annelated furobenzobicyclo[3.2.1]octadienes[1-7] by two photochemical key steps is presented: furo-benzobicyclo–[3.2.1]octadiene (**B**), obtained on irradiation of *o*–vinyl substituted styryl furan (**A**), was transformed *via* formyl derivative into new styryl benzobicyclo[3.2.1]octadienes (**C**) which by photochemical ring closure give the target molecules (**D**). The annelated bicyclo[3.2.1]octadiene derivatives are especially interesting for their rigid methano–bridged junction of two aromatic units at defined geometrical arrangement (Figure 1) and thereby as potentials for molecular clips construction.

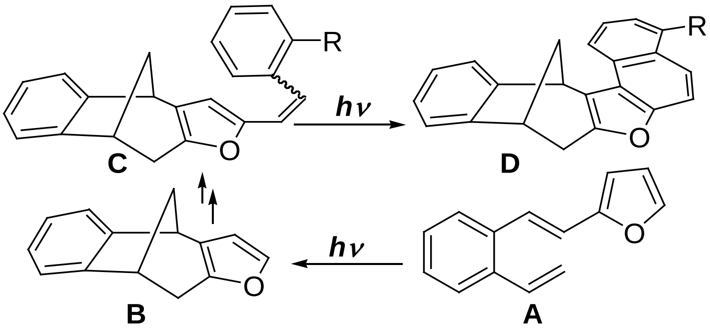

FIGURE 1

All new polycyclic structures are completely characterized by spectroscopic methods using modern techniques.

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TOPOLOGICAL INDICES OF GRAPHS WITH AND WITHOUT CUT EDGES

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Let G1 and G2 be simple undirected connected graphs. If there exists a bridge uv between graphs G1 and G2 as indicated on the figure below, we denote this graph as G1uvG2. If graphs G1, G2, and K2 share one common (cut) vertex u; then we denote this graph as G1uG2uK2. We look at the values of Wiener number W, modifed Wiener number W*, Szeged number Sz, modified Szeged number Sz* and Schultz index MTI of graph G1uvG2 and graph G1uG2K2. We prove the following inequalities:

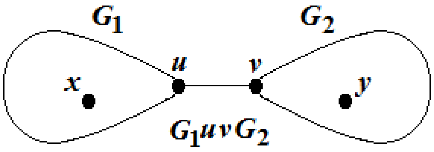
$W(G1uvG2) > W(G1uG2uK2)$,

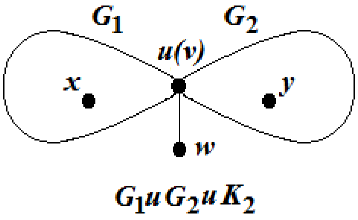
$Sz(G1uvG2) \geq Sz(G1uG2uK2)$,

$Sz^*(G1uvG2) \geq Sz^*(G1uG2uK2)$ and

$MTI(G1uvG2) > MTI(G1uG2uK2)$

for any simple connected graphs G1 and G2 with $|V(G1)|, |V(G2)| \geq 2$. For the modified Wiener number, we were able to prove only inequalities in case G1 and G2 are trees.[3]





Our motivation is to extend previous work (see, for example Refs. 1, 2) towards determining the graphs with extremal value of certain topological indices.

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MOLECULAR RECOGNITION THEORY IN DEVELOPMENT OF VACCINES

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Molecular Recognition Theory (MRT) is based on the finding that peptides specified by the complementary RNAs and DNAs bind to each other with higher specificity and efficacy. It is an applicable heuristic algorithm for the identification of possibly interacting amino acid pairs of short linear epitope/paratope sites. The limitation of MRT is that it cannot explain 3D protein interactions, but it can be a valuable starting point for more complex computational and experimental analysis. In order to achieve better efficacy the heuristic algorithm of molecular recognition has to be combined to several other procedures:

molecular hydropathy analyses,
secondary structure prediction methods, and
protein database search.

Described concept represents useful and simple set of procedures for the modulation and investigation of targeted peptide–receptor, *i.e.*, epitope–paratope interactions. It could also simplify experimental procedures, reduce the costs of the peptide synthesis, improve peptide structure modelling and identify possible targets relevant for the vaccine development and toxicology.

BUCHBERGER'S ALGORITHM AND ITS APPLICATIONS

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In this paper Buchberger's algorithm and its applications are described. Buchberger's algorithm (which can be viewed as a generalization of the Euclidean algorithm for computation of greatest common divisor of univariate polynomials and of Gaussian elimination for linear systems) transforms a given set of generators for a polynomial ideal into a Gröbner basis with respect to some monomial order. Some application of Buchberger's algorithm are: deciding equality of ideals, deciding membership of ideals, conversion of parametric equations, intersecting ideals, solving systems of polynomial equations, computation of greatest common divisor of multivariate polynomials... Since Buchberger's algorithm transforms given set of polynomials to a Gröbner basis which usually contains simpler polynomials that share certain characteristics with the original set of polynomials, it is always recommendable to try to compute a Gröbner basis if one encounters a problem formulated in terms of multivariate polynomial sets.

NITROSOBENZENES AS BUILDING–BLOCS FOR SUPRAMOLECULAR STRUCTURES

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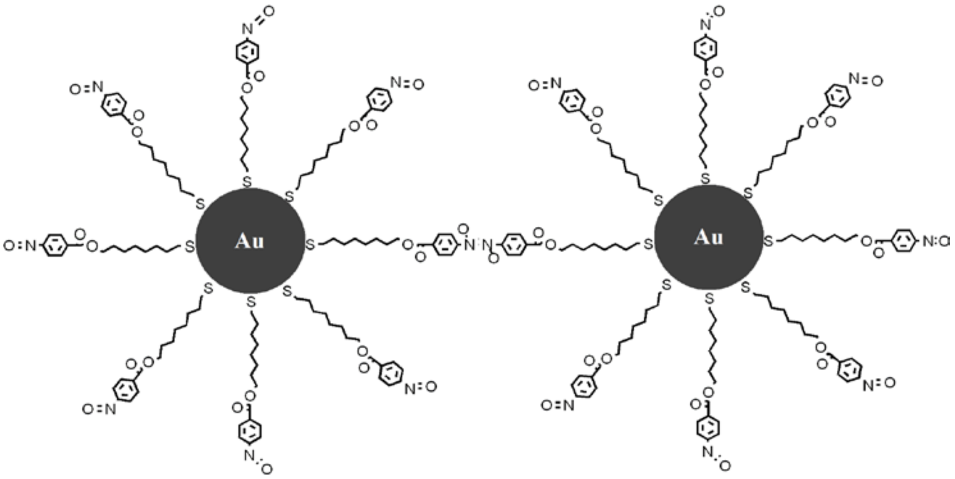
Property of nitrosobenzenes to form dimers, azodioxides, can be applied to construct supramolecular structures. The formation of nano–networks by using nitrosobenzene–coated colloid gold and the formation of 2D–organized mono– and bimolecular layers on the gold surface is presented.



ADRIATIC DESCRIPTORS – QSAR APPLICATIONS AND MATHEMATICAL PROPERTIES

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Some of the most famous molecular descriptors are bond additive, *i.e.*, they are calculated as the sum of edge contributions (Randić type indices, Wiener indices and its modifications, Szeged index, etc.). In this paper, the methods of calculations of bond contributions of these descriptors are analyzed. The general concepts are extracted and based on these concepts a large class of molecular descriptors is defined. These descriptors are named Adriatic indices.

Especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. They have been analyzed on the testing sets provided by International Academy of Mathematical Chemistry and it has been shown that they have good predictive properties in many cases. They can be easily encoded in the computer and it may be of interest to incorporate them in the existing software packages for chemical modeling. It is possible that they could improve various QSAR and QSPR studies.

Also, extremal graphs corresponding to one of these descriptors (Max–min rodeg index) have been analyzed. Many open problems are proposed.

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THE MODIFIED SCHULTZ POLYNOMIAL OF NANOTUBES AND NANOTORI COVERED BY C_4

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Let G be a connected graph. Suppose $d_G(a,b)$ denotes the length of a minimum path between vertices a and b of a graph G. The modified Schultz polynomial of G is defined as $W_*(G,x) = \sum_{\{a,b\}\subseteq V(G)} \deg_G a \ \deg_G b \ x^{d_G(a,b)}$.

In this paper we obtained the modified Schultz polynomial of some graph operations, and by using these results, we obtained the modified Schultz polynomial of nanotorus as well as of the nanotubes and nanotori covered by C_4.

Keywords: graph operation, modified Schultz polynomial**,** nanotube, nanotorus

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ENHANCED THERMAL TRANSPORT OF STRONGLY CORRELATED ELECTRONS

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The charge and heat transport of intermetallic compounds with Ce, Eu, and Yb ions are discussed using the periodic Anderson model with crystal field split f states. We show that the low–temperature properties are governed by the Fermi liquid (FL) laws with characteristic energy scale T_0 and that the high–temperature properties exhibit typical Kondoesque features, characterized by Kondo scale T_K.

Combining the FL theory and the high–temperature perturbation expansion we discuss modifications of the thermopower and the resistivity induced by pressure, doping or magnetic field. We show that the renormalization of transport coefcients in the FL regime can invalidate the Wiedemann–Franz law and enhance the power factor and the figure–of–merit. We also show that the thermoelectric response can be enhanced (or reduced) with respect to the predictions based on the single–impurity models that would lead to the same high-temperature behavior as the periodic Anderson model. Using these results, we discuss the thermoelectric response of some typical heavy fermions and valence uctuators. We explain the unusally large power factor and *slow crossover* observed in YbAl3, and the *rapid crossover* observed in YbInCu4.