EARLY DAYS OF THE MATH/CHEM/COMP MEETINGS

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The first MATH/CHEM/COMP Meeting was held in the Inter–University Centre of Postgraduate Studies in Dubrovnik on June 25–27, 1986. However, the name MATH/CHEM/COMP Meeting was not then used. What was to be the MATH/CHEM/COMP Meetings was incorporated into the 5th Research Seminar in Science, Technology and Environmental Policy. It was organized by the Center for Yugoslav–American Studies, Research and Exchanges at the Florida State University (Tallahassee) in cooperation with the Universities of Belgrade, Zagreb and Titograd and the Inter–University Centre in Dubrovnik. Besides people from economics, law, engineering and political sciences, the meeting was attended by about twenty mathematicians, physicists, chemists and computer scientists. Their participation was in the section Mathematics, Chemistry and Computer Science. This title inspired Chris Lacher to suggest the name for the future meetings MATH/CHEM/COMP. The proceedings from this meeting have been published by the Center for Yugoslav–American Studies, Research and Exchanges at the Florida State University in 1987. (V. Muljević, G.F. Macesich, eds.), but reports by Chris Lacher, DeWitt Sumners, David Edelson, Dragutin Svrtan, Darko Veljan, Ante Graovac appeared in a special issue of *Kemija u industriji* (1986) **35**:671–669, published by Croatian Society of Chemical Engineers and Technicians in Zagreb.

I was involved in early organization of this meeings by pure chance. So happened I have known Professor Vladimir Muljević since 1964. When he learned that I will be in the USA in autumn 1985, visiting Texas A&M University at Galveston, he invited me to visit the Centre for Yugoslav–American Studies in Tallahassee. I accepted his invitation and visited him there. Since Professor Doug Klein, whom I was visiting in Galveston, was invited to give talks at the Florida State University, we traveled together by car to Tallahassee. Besides visiting the Centre for Yugoslav Studies, I also visited Chris Lacher since I have known him from his visits to Zagreb. He and De Witt Sumners have known about the activities of the Centre for Yugoslav–American Studies and suggested that we join them with subsymposia on interaction between mathematics and natural sciences. After this initial meeting, we, with help from Ante Graovac, started to prepare the first meeting. The name MATH/CHEM/COMP has been in use since the second meeting, held on June 22–26, 1987. Some people did not like this name, but it remained unchanged ever since. The full title of these meetings is International Course and Conference on the Interfaces between Mathematics, Chemistry and Computer Science. All, but two, were held in Dubrovnik. These two were held in Rovinj, Istra, because of the attacks of Serbian and Montenegrain armies on Dubrovnik.

TWENTYFIVE YEARS OF THE MCC MEETINGS

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The Inter–University Centre (IUC) in Dubrovnik, founded in 1971 by Academician Ivan Supek, is an internationally recognized Centre for Advanced Studies in a broad range of scientific fields. It offered and continues to do so a fine framework for organization of the MATH/CHEM/COMP (MCC) Courses and Conferences Professors Dragutin Svrtan, Nenad Trinajstić, Darko Veljan and myself started in 1986.

The results achieved and their worldwide dissemination, reminiscence on some lecturers and also some problems the MCC meetings are facing will be presented. A personal view on how these meetings started is given at the end of this *Book of Abstracts*.

THE NUMBER OF CLOSED WALKS OF SOME INFINITE CLASS OF FULLERENES

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Let G be a simple graph. A closed walk is sequence $v_1v_2v_3\ldots v_mv_1$ of vertices of G where v_iv_{i+1} is an edge of G. In this paper, we compute the number of closed walks of an infinite class of (4,6)–fullerenes.

Keywords: (4,6)–fullerene, closed walk

I. Gutman, N. Trinajstić (1972) Graph theory and molecular orbitals: Total π–electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17**:535–538.

G.H. Fath–Tabar, M.J. Nadjafi–Arani, M. Mogharrab, A.R. Ashrafi (2010) Some inequalities for Szeged–like topological indices of graphs, *MATCH Commun. Math. Comput. Chem.*, **63**:145–150.

G.H. Fath–Tabar, A.R. Ashrafi, I. Gutman (2009) Note on Estrada and L–Estrada indices of graphs, *Bull. Acad. Serbe Sci. Arts Cl. Sci. Math. Natur.*, **139**:1–16.

THE ECCENTRIC CONNECTIVITY INDEX OF NANOSTRUCTURES

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Suppose u and v are vertices of a graph G. The topological distance $d(u,v)$ is defined as the length of the shortest path connecting u and v in G. For a given vertex u of $V(G)$ its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the diameter, $D(G)$, and the minimum eccentricity among the vertices of G is called the radius of G and denoted by $R(G)$. The eccentric connectivity index $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum_{u \in V(G)} \deg(u)\,\varepsilon(u),$$

where $\deg(u)$ denotes the degree of vertex u in G.[1,2] In this talk, we report our latest results on the problem of computing eccentric connectivity index of some new types of nanostructures.

1. V. Sharma, R. Goswami, A.K. Madan (1997) Eccentric connectivity index: A novel highly discriminating topological descriptor for structure–property and structure–activity studies, *J. Chem. Inf. Comput. Sci.*, **37**:273–282.
2. H. Dureja, A.K. Madan (2007) Superaugmented eccentric connectivity indices: New–generation highly discriminating topological descriptors for QSAR/QSPR modeling, *Med. Chem. Res.*, **16**:331–341.

DISTANCE IN THE NON–COMMUTATIVE GRAPH OF GROUPS

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Let Γ be an undirected connected graph without loops or multiple edges. The sets of vertices and edges of Γ are denoted by $V(\Gamma)$ and $E(\Gamma)$, respectively. For vertices x and y in $V(\Gamma)$, we denote by $d(x, y)$ the topological distance, *i.e.*, the number of edges on the shortest path, joining vertices x and y of Γ. Since Γ is connected, $d(x, y)$ exists for all $x, y \in V(\Gamma)$. The term Wiener number or Wiener index is nowadays in standard use in chemistry and is sometimes encountered also in the mathematical literature.[1] The Wiener index of the graph Γ is defined as the half sum of distances over all its vertex pairs (u, v):

$$W(\Gamma) = \frac{1}{2}\sum_{u,v \in V(\Gamma)} d(u,v)$$

For an edge $e(uv)$ of a graph Γ, let $n_u(e)$ denote the set of vertices of Γ lying closer to u than to v and $n_v(e)$ is the set of vertices of Γ lying closer to v than to u. The sets $n_u(e)$ and $n_v(e)$ play an important role in metric graph theory. Gutman defined the Szeged index, $Sz(\Gamma)$, of a graph Γ as:[2]

$$Sz(\Gamma) = \sum_{(uv)=e \in E(\Gamma)} |n_u(e)| \times |n_v(e)|$$

If Γ is a tree then $Sz(\Gamma) = W(\Gamma)$. We recall that is not true for any graph. Let G be a non–abelian group and let $Z(G)$ be the center of G. Associate with G a graph Γ_G as follows: take $G \backslash Z(G)$ as vertices of Γ_G and join its two distinct vertices x and y whenever $xy \neq yx$. Graph Γ_G is called the non–commutative graph of G.

In this paper we study some metric properties of Γ_G and compute the Wiener and Szeged indices of some linear groups.

1. A. A. Dobrynin, R. Entringer, I. Gutman (2001) Wiener index of trees – Theory and applications, *Acta Appl. Math.*, **66**: 211–249.
2. I. Gutman (1994) A formula for the Wiener number of trees and its extension to graphs cycles, *Graph Theory Notes of New York*, **27**:9–15.

PROBLEMS CONNECTED WITH THE AROMATICITY OF HYDROCARBONS AND HETEROCYCLES

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Linear correlations between
  (1) π–electron ring currents and
  (2) partitions of π–electrons
between various rings in benzenoids are possible for certain types of six–membered rings, as functions of their position on the dualist of the benzenoid.
In a joint publication with R. B. Mallion, these two numerical indices for local ring aromaticities were compared, and a third one introduced by Mandado, Bultinck and coworkers was also investigated for such fragmented linear correlations.
Among aromatic heterocycles, the most exciting are those predicted to be on the brink of stability either because of steric strain, or because of the agglomeration of electronegative heteroatoms.
Some predictions for possible new such aromatic heterocycles will be presented.

RING CURRENTS AND THE PCP RULE

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*According to the recently discovered PCP rule,[1] the intensity of cyclic conjugation in the five–membered rings of polycyclic conjugated hydrocarbons related to acenaphthylene and fluoranthene increases with the number of phenyl–cyclopentadienyl (PCP) fragments present in the molecule. The validity of this regularity was first observed by studying the energy effects of cyclic conjugation in the five–membered rings of these systems.[2,3] In order to show that the PCP rule is not an artifact of the method employed, it is necessary to confirm its validity by other approaches. We now show that the PCP rule is in perfect agreement with calculated topological π–electron ring–currents,[3] ostensibly an independent, quantitative, theoretical – albeit, it is here argued, likewise also *graph–theoretical* – measure of cyclic conjugation in the individual rings of polycyclic π–electron systems. In addition, we show that the molecular–structure dependency of the ring currents in acenaphthylene and fluoranthene congeners also agrees with other, earlier–established, regularities for cyclic conjugation.[4]

*A.T. Balaban, T.K. Dickens, I. Gutman, R.B. Mallion, *Croat. Chem. Acta.*, in press.

1. I. Gutman, J. Đurđević, A.T. Balaban (2009) *Polycycl. Aromat. Comp.*, **29**:3−11.
2. I. Gutman (2005) *Monatsh. Chem.*, **136**:1055−1069.
3. I. Gutman (2009) *Mathematical Modeling of Chemical Phenomena*, in: A. Graovac, I. Gutman, D. Vukičević (Eds.), *Mathematical Methods and Modelling for Students of Chemistry and Biology*: *Proceedings of the Conference Mathematical Methods in Chemistry, Split, Croatia, September 22−24, 2007*, Hum naklada d.o.o., Zagreb, pp. 13−27.
4. R. B. Mallion (2008) *Croat. Chem. Acta*, **81**:227−246.

THE COMPLEXITY OF CHEMICAL CLASSIFICATIONS

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Classification is one of the central means and goals of science. Chemical classification systems show an extraordinary complexity when compared to class structures commonly found in other disciplines: They involve two ground sets (substances and reactions) and normally lead to non–disjoint classes, which means that they can't be modeled as partitions on a set, a frequent mathematical image of classifications in science. Partition hierarchies, *e.g.* as those resulting from hierarchical clustering techniques, are not better suited for the task, since they require non–disjoint classes to be related by set–inclusion, which oftentimes is not the case in chemistry. We also note that chemical classifications over a set of substances are determined by relations among its elements established by a set of reactions, which suggests that a network approach is advisable over the often used *property vector space approach*.

Accounting for these considerations, we propose a mathematical formalization of the chemical approach to material classification as an optimization problem within a network model, and perform a preliminary analysis of its computational complexity.

QSAR ANALYSIS OF HETEROCYCLIC AMIDES AND QUINOLONES WITH POTENTIAL ANTITUMOR ACTIVITY

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QSAR models for predicting antitumor activity of heterocyclic amides and quinolones against MiaPaCa–2 (pancreatic carcinoma) and MCF–7 (breast carcinoma) cells were built. Complete dataset consisted of 59 compounds and several QSAR models with different predictive ability were derived using Volsurf software. Beside standard approaches for building QSAR models, the approach based on a small dataset of 10 compounds selected regarding the results of principal component analysis was tested. The latter approach was shown as successful and can be useful for planning future experiments in order to speed up and simplify the search for new drug candidates. Based on the derived QSAR models, the most important properties for compound’s antitumor activity against MiaPaCa–2 and MCF–7 cells were identified. New compounds, with potentially higher biological activity against MiaPaCa–2 and MCF–7 cells, were proposed. Their activities were predicted using the derived QSAR models and the proposed compounds were shown as promising antitumor candidates.

ADVANCES IN NITROSO CHEMISTRY

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The ambivalence of C–nitroso compounds to appear as monomers and/or dimers in solution as well as in solid state challenged chemists through last five decades. Here we represent our research in which this property is used as a model for investigation of solid state reaction mechanisms and phase transitions, structural and topochemical selectivity, behavior in self–assembly monolayers and applications in nanoscience.

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 have 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 at the B3LYP/6-31G* level in gas phase. We led a theoretical study 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, molecular orbital theory, regioselectivity, 1,3–dipolar cycloadditions

A. Padwa (1984) *1,3-Dipolar Cycloaddition Chemistry*, Wiley–Interscience, N.Y.
R.R. Kumar, S. Perumal, H.B. Kagan, R. Guillot (2006) *Tetrahedron*, **62**:12380.
P.K. Kalita, B. Baruah, P.J. Bhuyan (2006) *Tetrahedron Lett.*, **47**:7779.
M.P. Sibi, L.M. Stanley, T. Soeta (2006) *Adv. Synth. Catal.*, **348**: 2371.
W.J. Choi, Zh.D. Shi, K.M. Worthy, L. Bindu, R.G. Karki, M.C.Nicklaus, R.J. Fisher Jr., T.R. Burke (2006) *Bioorg. Med. Chem. Lett.*, **16**:5262.
M.M. Majireck, S.M. Weinreb (2006) *J. Org. Chem.*, **71**:8680.
R. Huisgen, G. Szeimies, L. Mobius (1966) *Chem. Ber.*, **99**:475.
W. Broeckx, N. Overbergh, C. Samyn, G. Smets, G. L’abbe (1971) *Tetrahedron*, **27**:3527.
R.G. Parr, L. von Szentpaly, S.J. Liu (1999) *J. Am. Chem. Soc.*, **121**:1922.
R.G. Parr, W. Yang (1989) *Density Functional Theory of Atoms and Molecules*, Oxford University Press, N.Y.
R.G. Parr, W. Yang (1984) *J. Am. Chem. Soc.*, **106**:4049.
P.K. Chattaraj, S. Nath, A.B. Sannigrahi (1994) *J. Phys. Chem.*, **98**:9143.
L.R. Domingo, M.J. Aurell, P. Perez, R. Contreras (2002) *J. Phys. Chem. A*, **106**:6871.
I. Fleming (1976) *Frontiers Orbitals and Organic Chemical Reactions*, Wiley, London.

CARBONMONOXIDE ADSORPTION ON 4–, 5– AND 6–ATOM CAGE BORON MICROCLUSTERS

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Electronic structure of $B_mH_{m-n}(CO)_n$ ($m = 4 - 6$, $n \leq m$) complexes have been investigated *via* performing Density Functional Theory with B3LYP functional and 6 – 311g basis.[1] Some of the computed results of our continuing study on boron–molecule systems will be presented. The total energies, binding energies, HOMO–LUMO energy gaps, frequencies, electronic states, structural parameters and point groups of the structures have been obtained for cage forms of 4–, 5– and 6–atom boron clusters in the B_m–centered complexes. The B_4, B_5 and B_6 structures in the complexes have been initially prepared in pyramidal, bipyramidal and square bipyramidal forms, respectively. The B_4 with 2 or 3 CO molecules cannot stay in its pyramidal form and displays a rhombic like configuration. The B_5 keeps its trigonal bipyramidal structure with 1, 2 and 3 CO molecules but it is converted into a square pyramidal form with 4 and 5 CO molecules. The B_6 for up to 5 CO molecules remains in the square bipyramidal structures, however it changes its form to a prism geometry in $B_6(CO)_6$. Various conformations of CO on the B_6 have been particularly studied for both sites of CO as O attached and C attached on the B atoms. In the $B_6(CO)_6$ cluster, the B_6 prefers to transforms itself into a prism structure with 1 and 2 B–O bonds but the cage square bipyramidal form of the B_6 keeps its structural morphology with 3, 4, 5 and 6 B–O neighbouring bonds. It is also observed that the lower–lying structures have been observed by increasing B–C neighbouring conformations. Moreover, the structural distortion mechanism can easily dominate in the given complexes not containing any hydrogen atom.

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M. J. Frisch *et al.* (2004) *Gaussian 03, revision D.01*, Gaussian, Inc., Wallingford, CT, USA.

ORDINAL STATISTICS TO ANSWER ORDINAL QUESTIONS

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Comparing distributions there are two basic research questions to be considered.
The first is:

Do the two distributions differ?

And the second:

To what extent is this true?

Since school grades represent an ordinal scale, in our contribution we will apply ordinal statistics to answer these ordinal questions.

The first research question will be answered by the standard Mann–Whitney–Wilcoxon (MWW) test.

The second research question will be addressed using *ordinal dominance graph* (ODG) and *directed dissimilarity* $d = P(X>Y)–P(X<Y)$. Properties of the directed dissimilarity d will also be discussed: antisymmetric, vanishes on the diagonal, $|d|$ is dissimilarity, *etc*.

We intend to incorporate presented ordinal statistics in the **ALA Tool**, *i.e.*, Assessment of/for Learning Analytic Tool for gathering and analysis of grades in upper secondary education in Slovenia. Real data on student gradings in upper secondary education in Slovenia will be analyzed. We will answer the research question:

Are the students that select science optional subjects (Chemistry, Physics) better achievers in overall Matura exam?

We hope to find some application of presented concepts also in the field of Chemistry.

DNA INTERCALATION OF AFLATOXIN B_1 AND RELATED MICOTOXINS IS ENHANCED THROUGH PREORGANIZED ELECTROSTATICS OF THE EVOLUTIONARILY CONSERVED FUROFURAN REGION

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Aflatoxin B_1 and related furofuran micotoxins produced by the common molds of *Aspergillus* are of great interest due to their role in the etiology of human liver cancer. After intake they get epoxidized by cytochrome P450 to corresponding ultimate carcinogens which alkylate DNA, evidently after intercalation. Aflatoxin B_1 *exo*–8,9–epoxide intercalation free energy of –4.1 and –4.9 kcal/mol was calculated using Molecular Dynamics (MD) simulations in conjunction with Linear Interaction Energy (LIE) and Linear Response Approximation (LRA) methods, respectively, and compares favorably with the range of –3.9 to –4.9 kcal/mol obtained experimentally using various techniques and nucleobase sequences. Moreover, to provide an insight into interactions responsible for intercalation, the electrostatic, dispersion, preorganization as well as various group contributions to the calculated free energy were explicitly determined. The furofuran region is electrostatically preorganized to bind DNA, which has the potential to explain, why this structural element was evolutionarily conserved in a variety of micotoxins. On the other hand, the large planar body enhances intercalation solely through dispersion interaction, which again explains, why this region of related micotoxins could have been evolutionarily optimized in a different way. Finally, comparing generation of Near Attack Configurations (NAC) during the course of MD simulations involving charged and uncharged aflatoxin B_1 *exo*–8,9–epoxide, respectively, revealed that preorganized electrostatics plays a vital role also in the subsequent chemical step and speeds up the corresponding alkylation by a factor of 4.5.

GENERATING CUBIC GRAPHS (AGAIN)

Gunnar BRINKMANN, Jan GOEDGEBEUR

LINEAR TRANSFORMATIONS IN CRYSTALLOGRAPHY

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Linear transformations are a basic mathematical tool in crystallography. They are mostly used and studied in the forms of coordinate transformations and of symmetry operations. The course will cover both applications.

Symmetry operations are used to classify crystals. The point group elements are linear transformations and, provided a basis is chosen, can be represented by matrices. The translations are not linear transformations, but all the symmetry operators can be represented by one matrix for the linear transformation part and one column–matrix representing the translation vector. The first part of the course will cover symmetry operators and their usage.

An often used coordinate transformation is the rotation of the coordinate system, but this is by far not the only coordinate transformation useful in crystallography. We shall explore various examples of the coordinate transformations occurring in crystallographic contexts, including the change of basis for the usual three–dimensional space when shifting from descriptions of crystals in direct space to the descriptions in reciprocal space.

The prerequisite for the course is a basic knowledge about finite–dimensional vector spaces and their bases, linear operators and their matrix representations, as they are usually covered in pregraduate courses in linear algebra in the first years of studies in mathematics, physics or chemistry.

CLIMATEGATE, GLOBAL WARMING AND BAD SCIENCE

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In 1988 James Hansen (NASA Goddard Institute for Space Studies) gave testimony on climate change to US congressional committees postulating that if global temperature rises 0.4^0C above 1950–1980 mean for few years, it is *smoking gun* pointing to human–caused global warming. In 1998, Michael Mann (Penn State University, USA), published paper that claims unprecedented global warming in 1990’s not seen in the last 1000 years. In November 2009, several thousands of emails, documents and source codes from Climate Research Unit (CRU) at University of East Anglia, have been leaked (Climategate), indicating widespread miss–use of original data, scientists affecting peer reviewing system of major journals to prevent publications that do not support anthropological global warming (AGW) theory, not releasing data and computer code for an independent review of their findings and deleting original data. Following the release of the emails, director of CRU, Phil Jones had to resign, was subject to two enquires by the governmental and scientific bodies in UK, Michael Mann has been subjected to enquiry by the Penn State University, and Al Gore called to be testified in front of the US Senate Committee for his miss–interpretations of graphs showing *correlation* between the temperature trends and CO_2 that has won him Nobel prize and Oscar for the movie *An Inconvenient Truth*. All the predictions of the models have failed to materialize. As a consequence of AGW theory, CO_2 and Carbon have been declared as pollutants, redefining well established chemical facts:

1. CO_2 is fundamental for life – every breath out releases CO_2 being integral part of all biochemical processes inside human body, it is the key part of photosynthesis that produces Oxygen,
2. Carbon is key element of our DNA, amino acids and proteins, and no drug molecule would be possible without Carbon.

The climate models fail all *good scientific practices* and software producing models fail all software quality control audits.

BenzoGraphiX – A COMPUTER SYSTEM FOR STUDYING BENZENOIDS

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A polyhex hydrocarbon is a connected set of regular hexagons such that two different hexagons either share an edge or are disjoint. Should this polyhex be represented on a hexagonal lattice, it is called benzenoid. Benzenoids are extensively studied in mathematical chemistry. The system BenzoGraphiX (BGX) allows a fast computation of a series of molecular descriptors for a benzenoid that is drawn interactively, and also has a heuristic optimization routine to identify optimal or near optimal configuration. The BGX optimization will attempt to find a benzenoid with maximum or minimum value for the molecular descriptor under study by keeping fixed the number of hexagons. Compared to generic systems such as AutoGraphiX, BGX takes advantage of the particular structure of a benzenoid to speed up the computations. Another advantage is that each hexagon is associated to a position on the plane, which allows studying molecular descriptors that rely on the way the molecular graph is drawn (as opposed to invariants). For example, any molecular descriptor based upon the physical distance between pairs of atoms could be considered, a capability that may be of interest. The system will be presented as well as some preliminary results.

STABILITY OF FULLERENES AND FULLERANES TOWARD CORPUSCULAR AND ELECTROMAGNETIC RADIATION

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The stability of C_{60} and C_{70} fullerenes in the interstellar medium deposited on dust surface or embedded in meteorites and comets has been simulated with γ irradiation and with He^+ ion bombardment. It is shown by vibrational spectroscopy that a γ radiation dose of 2.6 MGy (1Gy = 1 joule absorbed energy/kg) causes partial oligomerization of both C_{60} and C_{70} fullerenes. Oligomers are made by fullerene cages chemically connected with each other which can yield back free fullerenes by a thermal treatment. The amount of irreversibly polymerized fullerenes caused by 2.6 MGy as deduced as the toluene insoluble fraction has been determined as 1.7% and 15% by weight respectively for C_{60} and C_{70} fullerene. The radiation dose generated by radionuclides decay and expected to be delivered to fullerenes buried at a depth of more than 20 m in comets and meteorites is about 3 MGy per 10^9 years. Since fullerenes are by far resistant to such radiation dose they can survive for largely more than 5×10^9 years inside comets and meteorites and in fact have been detected inside certain carbonaceous chondrites. On the other hand, the direct exposure of fullerenes to cosmic rays, for instance when they are adsorbed or deposited on the surface of carbon dust, corresponds to the delivery of a radiation dose comprised between 30 and 65 MGy/10^9 years. Experimental bombardment of both C_{60} and C_{70} fullerenes for instance with He^+ ions has shown that the complete amorphization occurs at about 250 MGy. Thus in about 3.8×10^9 of years exposure to cosmic rays a complete amorphization is expected.

F. Cataldo, S. Iglesias–Groth, A. Manchado (2009) *Mon. Not. Roy. Astron. Soc.*, **400**:291–298.
F. Cataldo, S. Iglesias–Groth, A. Manchado (2009) *Mon. Not. Roy. Astron. Soc.*, **394**:615–623.
O. Ori, F. Cataldo, S. Iglesias–Groth, A. Graovac (2010) Topological modeling of hydrogenated fullerenes, Chapter 12, in: *Fulleranes: the Hydrogenated Fullerenes*, Springer, Berlin.

FULLERENE SOLUBILITY IN FATS AND THEIR POTENTIAL APPLICATION AS ANTINEOPLASTIC AGENTS

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One peculiarity of fullerenes is their high level of unsaturation. For instance C_{60} possesses 30 weakly conjugated double bonds. For a number of reasons, these double bonds are readily reactive with free radicals. C, N, S, O centred radicals are able to add on the fullerene double bonds leading to neutral adducts. For instance, up to 16 bulky benzyl radicals and up to 34 small methyl radicals can be added on a *single* C_{60} fullerene molecule. For this peculiar property the fullerenes and in particular C_{60} fullerene, have been defined as *free radical sponges*.

Experiments with a series of molecules which act as free radical acceptors have clearly shown the possibility to inhibit the growth of tumors. However, all the radical scavengers commonly known as antineoplastic are able to accept just one or two free radicals per molecule. Instead, C_{60} fullerene is able to accept from 16 to 34 free radicals/molecule. This may imply both the possibility to have fullerenes effective in the inhibition of tumor growth at very low dosages or to have a very powerful effect in tumor growth inhibition.

We have discovered and patented (only in Italy at present) that fullerenes are soluble in fatty acid esters. Not only they are soluble in methyl and ethyl esters of fatty acids, the fullerenes are soluble even in the glycerol esters of fatty acids thus even in the common olive, soybean, sunflower, peanut, linseed and castor oils. Additionally fullerenes are soluble in butter and margarine, and also in free fatty acids such as oleic acid and molten stearic acid. This discovery paves the way to use fats as a vehicle to deliver fullerenes *in vivo*. An adequate experimentation should be organized to make tests both *in vitro* and *in vivo*.

F.Cataldo, T. Braun (2007) *Fullerenes Nanot. Carbon Nanostruct*., **15**:331–339.
F. Cataldo, T. Da Ros (Eds.) (2009) *Medicinal Chemistry and Pharmacological Potential of Fullerenes and Carbon Nanotubes*, Springer, Berlin.
F.Cataldo, Italian Patent N° 1,372,085 filed 19th January 2007.

STONE–WALES WAVES IN GRAPHENE LAYERS

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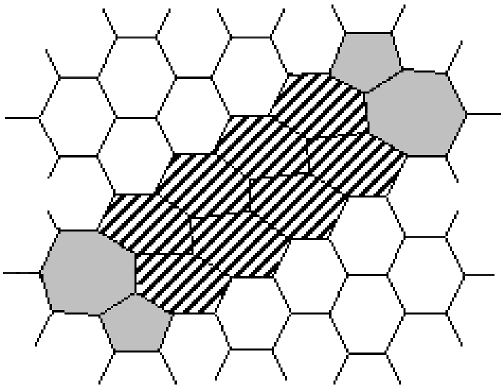
Stone–Wales local rearrangements of the graphene hexagonal mesh generate two pentagonal and two heptagonal rings in place of four proximal hexagons. As presented in this paper, these topological alterations may be easily iterated along both graphene lattice directions and propagate the Stone–Wales rearrangements on larger distances, a topological effect we call Stone–Wales waves. Wiener index, applied as a hypothetical pure topological potential of the graphenic lattice, describes graphene lattice reactions to these propagating Stone–Wales waves. Topologically, Stone–Wales waves are equivalent to non–local generalized Stone–Wales transformations of graphene layers. Sequence of Stone–Wales rearrangements is able to generate nanocones on the graphene layer. In order to simplify the studies they are mainly carried out in the dual topological space.



Keywords: graphene, Stone–Wales waves, Wiener index

CHARGED PARTICLES IN SPHERICAL CONFINEMENTS

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Recent advances in theory of systems composed of charged particles subject to potentials with spherical symmetry are reviewed. In particular, the following subjects are discussed:

1. Full configuration interaction calculations on two– and three–electron harmonium atoms;
2. Spherical Yukawa crystals;
3. Spherical Coulomb crystals with power–law confining potentials;
4. Spherical Coulomb crystals with arbitrary confining potentials.

Illustrative examples demonstrating the interplay between theoretical predictions and the results of numerical simulations are provided.

THE REHYBRIDIZATION EFFECT ON CYCLIC COMPOUNDS

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Ab initio RHF and density functional B3LYP and B3PW91 calculations have been carried out on some cyclic and acyclic compounds of group IVA. The results of structural investigation show that all cyclic molecules, X_3H_6, have planar structures. The X–X bond lengths are slightly shorter than normal, while X–X–X internuclear angles of 60° are much smaller than the tetrahedral angle of 109.5°. In the acyclic compounds, X_3H_8, bond lengths and angles are near the normal tetrahedral bond lengths and angles. Vibrational analysis carried out on the RHF, B3LYP and B3PW91 optimized structures using 6–31++G** basis set, characterizes all of the optimized structures as minima on the potential energy surface without any negative mode. NBO analysis shows that in acyclic compounds X atoms have almost sp^3 hybridization in their bonds with H atoms. This explains the relatively high acidity of cyclic compounds versus acyclic compounds. The calculated NMR shielding constants show that the hydrogens of the cyclic compounds are more acidic than those of the acyclic compounds because the external X–H bonds of the cyclic compounds have more *s* character than those of the acyclic compounds. These results indicate some important differences in rehybridization capability between some cyclic and acyclic compounds of C, Si, and Ge.

SPACE FULLERENES: COMPUTER SEARCH FOR NEW FRANK–KASPER STRUCTURES*

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A fullerene is a 3–valent polyhedron whose faces are hexagons and pentagons (so, 12 of them). A fullerene is said to be Frank–Kasper if its hexagons are adjacent only to pentagons. There are four such fullerenes: with 20, 24, 26 and 28 vertices.

A space fullerene is a 4–valent 3–periodic tiling of R_3 by Frank–Kasper fullerenes. Space fullerenes are interesting in Crystallography (metallic alloys, zeolites, clathrates) and in Discrete Geometry. 27 such structures, all realized by alloys, were known before this work.

We enumerated the space fullerenes with a small fundamental domain under their translation groups: 84 structures with at most 20 fullerenes in the reduced unit cell (*i.e.*, by a Biberbach group) are found. 13 among them are known ones, including A_{15}, Z, C_{15} and 4 other Laves phases.

Moreover, there are 16 new proportions of fullerenes with 20, 24, 26, 28 vertices in the unit cell. Three among them – proportions (6 : 6 : 4 : 0), (6 : 8 : 4 : 0), (7 : 4 : 2 : 2) – provide first conterexamples to a conjecture by Rivier–Aste (1996) and to the old conjecture by Yarmolyuk–Kripyakevich (1974) that the proportion should be a conic linear combination of proportions (1 : 3 : 0 : 0), (2 : 0 : 0 : 1), (3 : 2 : 2 : 0) of A_{15}, C_{15}, Z, respectively.

So, a new challenge to practical Crystallography and Chemistry is to check the existence of alloys, zeolites, or other compounds having one of 71 new geometrical structures.

*It is a joint work with Mathieu DUTOUR and Olaf DELGADO.

SHELL–POLYNOMIALS IN NANOSTRUCTURES

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Shell–polynomials *P*(ShM,*x*) are counting polynomials derived from topological square matrices by applying Diudea's Shell–matrix operator. They describe a graph property *P*(*G*) in terms of a sequence of numbers so that the exponents express the extent of its partitions while the coefficients are related to the number of partitions of a given extent. Basic definitions and examples are given for the Shell–distance and Shell–degree–distance polynomials in two classes of T(4,4)[c,n] tori (Fig. 1).

Figure 1. Tori of the series T(4,4)S[5,n] (left) and T(4,4)R[5,n] (right)

M.V. Diudea, I. Gutman, L. Jäntschi (2002) *Molecular Topology*, NOVA, N.Y.
M.V. Diudea (2009) Cluj polynomials. *J. Math. Chem*., **45**:295–308.
M.V. Diudea, M.I. Topan, A. Graovac (1994) Layer matrices of walk degrees, *J. Chem.Inf. Comput. Sci*., **34**:1072–1078.
M.V. Diudea, O. Ursu (2003) Layer matrices and distance property descriptors, *Indian J. Chem*., **42A**:1283–1294.
M.V. Diudea, A.R. Ashrafi (2010) Shell–polynomials and Cluj–Tehran index in tori T(4,4)S[5,n], *Acta Chim. Sloven*., submitted.
M.V. Diudea, A. Iranmanesh (2010) Hosoya–Diudea polynomials revisited, *MATCH Commun. Math. Comput. Chem*., submitted.

NEW BOUNDS ON SOME FULLERENE INVARIANTS

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We establish a new lower bound on the diameter and a new upper bound on the bipartite edge frustration of a fullerene graph that are both proportional to the square root of the number of vertices. The new bounds are then used to settle in affirmative a conjecture on the smallest eigenvalue of a fullerene graph and to improve the existing upper bounds on the saturation number of fullerenes.

CUBIC POLYHEDRAL RAMANUJAN GRAPHS WITH FACE SIZE NO LARGER THAN 6

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A 3–valent plane graph is said to be of positive curvature if its face sizes belong to the interval [3,6]. Thus, such graphs, which generalize fullerenes belong to 19 classes according to (p3,p4,p5). A 3–valent graph is called Ramanujan if its eigenvalues a, besides 3 and possibly –3, $|a| \leq 2\sqrt{2}$.

We report here on ongoing work on the enumeration of Ramanujan 3–valent plane graphs of positive curvature. We give several bounding results on Ramanujan graphs that allow us to get an upper bound of 138 on the size of the vertex set. We also prove that for any subinterval I of [–3,3] there is a finite number of graphs of positive curvature having no eigenvalues in I.

The obtained results, based on computer computations, are then presented.

CONTRIBUTIONS TO THE THEORY OF FLUORANTHENES

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In our earlier studies of the π–electron properties of fluoranthenes, we established two general regularities, named *PCP* (= **p**henyl–**c**yclo**p**entadienyl) *rule* and *linear rule*. According to the *PCP* rule, a six–membered ring connected to the five–membered ring by a single carbon–carbon bond (= *PCP* constellation) increases the intensity of cyclic conjugation in the five–membered ring. According to the linear rule, a six–membered ring in linear constellation to the five–membered ring (*i. e.*, separated from the five–membered ring by another six–membered ring, but not in *PCP* constellation) decreases the intensity of cyclic conjugation in the five–membered ring. These rules were first observed by considering the energy effects of cyclic conjugation. Eventually, the rules were corroborated by other methods (*e.g.*, by ring currents, carbon–carbon bond lengths, etc).

We now report our studies of the *PCP* and linear rules, done by examining the respective NICS (nucleus–independent chemical shift) values. As a kind of surprise, we find that the NICS values of the five–membered ring of fluoranthene congeners precisely follow the *PCP* and linear rules, ***except*** that according to this criterion, rings in *PCP* constellation ***decrease***, and rings in linear constellation ***increase*** the "aromaticity" (as predicted by NICS) of the five–membered ring. This phenomenon is one more example that "aromaticity" assessed by energetic, geometric, and magnetic criteria might significantly differ.

ON THE SYMMETRY OF FULLERENES

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A Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix $M = [d_{ij}]$, where for $i \neq j$, d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for distinct nuclei.

In this paper, we first compute the Euclidean graph matrix of an infinite class of fullerenes. By using this matrix, the topological symmetry group of this class of fullerenes is computed.

Keywords: Euclidean graph, symmetry, fullerene

A.R. Ashrafi (2005) *MATCH Commun. Math. Comput. Chem.*, **53**:161–174.
A. R. Ashrafi (2005) *Chem. Phys. Lett.*, **406**:75–80.
G.S. Ezra (1982) *Symmetry Properties of Molecules*, *Lecture Notes in Chemistry*, **28**, Springer, Berlin–Hidelberg.
A.R. Ashrafi, M. Hamadanian (2003) *Croat. Chem. Acta*, **76**:299–303.

ON WIENER INDEX OF NANOSTRUCTURES

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The Wiener index of a graph G is defined as:
$W(G) = 1/2 \sum_{x,y \in V(G)} d(x,y)$,
where $V(G)$ is the set of all vertices of G and for $x, y \in V(G)$, $d(x, y)$ denotes the length of a minimal path between x and y. In this talk the latest results on computing Wiener index of nanostructures are reported.

Keywords: Wiener index, fullerene, nanotube

M.V. Diudea (2002) Hosoya Polynomial in Tori, *MATCH Commun. Math. Comput. Chem.*, **45**:109–122.

M.V. Diudea, E.C. Kirby (2001) The Energetic Stability of Tori and Single Wall Tubes, *Fullerene Sci. Technol.*, **9**:445–465.

S. Yousefi, A.R. Ashrafi (2006) An Exact Expression for the Wiener Index of a Polyhex Nanotorus, *MATCH Commun. Math. Comput. Chem.*, **56**(1):169–178.

THE ESTRADA INDEX OF SOME FULLERENES

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Suppose *G* is a graph and $\lambda_1, \lambda_2, \ldots$ are the eigenvalues of *G*. The Estrada index EE(*G*) of the graph *G* is defined as the sum of e^{λ_i}. In this paper we compute the Estrada index of an infinite class of (3,6)–fullerenes.

Keywords: Estrada index, (3,6)–fullerene, eigenvalues of graph

A.R. Ashrafi, F. Rezaei (2007) PI index of polyhex nanotori, *MATCH Commun. Math. Comput. Chem.*, **57**:243–250.

I. Gutman, N. Trinajstić (1972) Graph theory and molecular orbitals: Total π–electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17**:535–538.

GENERATING FUNCTIONS AND BIJECTIONS FOR BI–WALL DIRECTED POLYGONS

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In this talk, we define a new family of polyominoes. The name of the family is *bi–wall directed polygons.* A bi–wall directed polygon is a directed animal bounded by such a self–avoiding polygon which has the following property: when one goes along the polygon in the clockwise direction (starting and ending at the lower left corner of the source cell), once the first leftward step has been made, an upward step is made never more.

Bi–wall directed polygons are interesting because they are both a superset of column–convex directed polygons and a superset of diagonally convex directed polygons. Also, when a bi–wall directed polygon is reflected about the line $y = x$, the resulting figure is a bi–wall directed polygon again.

For general directed animals, the area generating function is given by the simple formula

$$\frac{1}{2}\cdot\left(\sqrt{\frac{1+q}{1-3q}}-1\right)$$

(found by Dhar, Phani and Barma in 1982), but the perimeter generating function remains elusive.

For bi–wall directed polygons, the area generating function is

$$\frac{q(1-2q)}{1-4q+3q^2+q^3}$$, and the perimeter generating function is

$$x\cdot\left(1-2x-\sqrt{1-6x+5x^2}\right).$$

(We obtained these results using the Temperley methodology.)

At present, bi–wall directed polygons are the largest class of directed animals for which the perimeter generating function is known.

The coefficients of the above–stated generating function

$$\frac{q(1-2q)}{1-4q+3q^2+q^3}$$

can be found in *The On–Line Encyclopedia of Integer Sequences*, maintained by N.J.A. Sloane. Namely, the number of n–celled bi–wall directed polygons is also the number of certain lattice paths with $n – 1$ steps. To be specific, the paths in question *live* in the strip $0 \le y \le 5$, end on the line $y = 0$, and are allowed to make three kinds of steps: (1, –1), (1, 0) and (1, 1). We found a bijection between bi–wall directed polygons and the paths just described. We also defined some other bijections. One of those bijections links directed column–convex polygons with paths which are very similar to those just described, the only difference being that the horizontal strip is $0 \le y \le 3$.

EXPLORING HOMO–LUMO MAPS

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Recently, we introduced a graphical tool for investigating spectral properties of graphs that we call **HOMO–LUMO maps**. On a HOMO–LUMO map a graph G is represented by the point with (λ_h, λ_l) coordinates, where, roughly speaking λ_h and λ_l are the two middle eigenvalues of G. The difference ($\lambda_h - \lambda_l$) is the well–known HOMO–LUMO gap in Hückel theory. Therefore it is surprising that although the middle eigenvalues have clear significance in mathematical chemistry, not much attention has been paid to them in spectral graph theory. It turns out that the HOMO–LUMO map is a well suited tool for investigating families of graphs, such as molecular trees, fullerenes, *etc.*, where extremal points or the patterns that appear may raise interesting questions. We will explore various regions of HOMO–LUMO maps. For example, all bipartite graphs belong to the line $\lambda_h + \lambda_l = 0$, but there are other graphs with this property. We call them pseudo–bipartite graphs. Graphs belonging to some other special lines will be explored.

P.W. Fowler, T. Pisanski (2010) HOMO–LUMO maps for chemical graphs, *MATCH Commun. Math. Comput. Chem.*, **64**:373–390.
P.W. Fowler, T. Pisanski (2010) HOMO–LUMO maps for fullerenes, *Acta Chim. Slov.*, in press.

SOME CLASSES OF GEOMETRIC–ARITHMETIC INDICES

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The geometric–arithmetic index is a topological index defined as:

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

where degree of vertex u is denoted by d_u. Now we define a new version of GA index as:

$$GA_5(G) = \sum_{e=uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}, \text{ where } \delta_u = \sum_{uv \in E(G)} d_v \ .$$

The goal of this paper is to further the study of the GA_5 index.

M.V. Diudea, (Ed.) (2001) *QSPR/QSAR Studies by Molecular Descriptors*, Nova, N.Y.
B. Furtula, A. Graovac, D. Vukičević (2009) *Discrete Appl. Math.*, **157**:2828.
D. Vukičević, B. Furtula (2009) *J. Math. Chem*., **46**:1369.
B. Zhou, I. Gutman, B. Furtula, Zh. Du (2009) *Chem. Phys. Lett.*, **482**:153.
M.A. Hosseinzadeh, M. Ghorbani (2009) *J. Optoelectron. Adv. Mater*., **11**:1671.

EXCEPTIONALLY HIGH STABILITY OF SOCCER BALL C_{60} AMONG SPHERICALLY POLYHEDRAL π–ELECTRON NETWORKS

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It has been established that the soccer ball–shaped fullerene C_{60} has exceedingly high stability of conjugated π-electron network among the 1812 spherical isomers composed of 20 hexagons and 12 pentagons with all the same vertex–degree of three irrespective of the grade of accuracy of the theory adopted.

The present author has developed the theory of topological symmetry by which the secular determinant of a highly symmetrical π–electron network can be factored out.[1] In this report this technique was applied to various spherically polyhedral networks mostly of regular and semiregular polyhedra. Although the valency of some networks are four and five, those data are included for formal discussion. The essence of the results are given in the Table 1.

Table 1.

Polyhedron	Code	V	valency	open (×) closed (○)*		HOMO degeneracy	$^{\#}$K
Cuboctahedron	$(3,4)^2$	12	4	×	△	3	32
Truncated tetrahedron	$3,6^2$	12		○	△	2	8
Truncated cube	$3,8^2$	24		×	△	5	32
Truncated octahedron	$4,6^2$	24		○	○	3	169
Rhombicuboctahedron	$3,4^3$	24	4	×	△	4	1088
Icosidodecahedron	$(3,5)^2$	30	4	×	×	4	2048
Truncated cuboctahedron	4,6,8	48		×	△	4	16384
Truncated dodecahedron	$3,10^2$	60		○	△	10	2048
Truncated icosahedron	$5,6^2$	60		○	○	5	12500

*× = antibonding; △ = nonbonding; ○ = bonding; $^{\#}$K = perfect matching number

By using these results the exceptionally high stability of the soccer ball–shaped C_{60} fullerene network will be discussed.

1. H. Hosoya, Y. Tsukano (1994) *Fullerene Sci. Tech.*, **2**:381.

THE MULTIPLICATIVE WIENER INDEX OF SOME NANOTUBES AND NANOTORI

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Let G be a simple graph with the set of vertices $V(G) = \{v_1,....,v_n\}$. The distance matrix $D(G)$ of G is a square matrix of order n, whose entry d_{ij} is the distance between vertices v_i and v_j in the graph G. The multiplicative Wiener index introduced by Gutman et *al.*[1] is equal to the product of the distances between all pairs of vertices of the underlying molecular graph G:

$$\pi(G) = \prod_{i<j} d_{ij} \cdot$$

In this paper, we compute this index for some nanotubes and nanotori by considering them as Cartesian products of paths and cycles. Also we compute this index for some composite graphs.

1. I. Gutman, W. Linert, I. Lukovits, Ž. Tomović (2000) The Multiplicative Version of the Wiener Index, *J. Chem. Inf. Comput. Sci.* **40**:113–116.

ECCENTRIC CONNECTIVITY POLYNOMIALS OF SOME CLASSES OF FULLERENES

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The eccentric connectivity polynomial of a molecular graph G is defined as:
$\mathrm{ECP}(G, x) = \Sigma_{x \in V(G)} x^{\mathrm{ecc}(x)}$,
where $\mathrm{ecc}(x)$ is the length of a maximal path connecting x to a vertex of G.
In this paper this polynomial is computed for some families of fullerenes.

Keywords: fullerene, eccentric connectivity polynomial, eccentric connectivity index

A.R. Ashrafi, M. Ghorbani, M. Jalali (2009) *J. Optoelectron. Adv. Mater.*, **3**:823–826.
S. Sardana, A.K. Madan (2001) *MATCH Commun. Math. Comput. Chem.*, **43**: 85–98.
S. Gupta, M. Singh, A.K. Madan. (2002) *J. Math. Anal. Appl.*, **266**:259–268.
B. Zhou, Z. Du (2010) *MATCH Commun. Math. Comput. Chem.*, **63**:181–198.
T. Došlić, M. Ghorbani, M.A. Hosseinzadeh (2010) *Utilitas Mathematica*, in press.

MODELING OF OZONE AND HYDROGEN PEROXIDE IN AIR

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Ozone (O_3) and hydrogen peroxide (H_2O_2) volume fractions were calculated using the Master Mechanism (MM) model, author S. Madronich (NCAR, Boulder, CO, USA). MM is an atmospheric *box* model program for calculating the time evolution of atmospheric composition from initial amounts of atmospheric gases under chosen or varying conditions using reaction rate data and other physical parameters. The photolysis coefficients were calculated using the Tropospheric Ultraviolet Visible (TUV) program of the same author. The present study analyzes the relationships between different initial conditions (air temperature, relative humidity, levels of some atmospheric pollutants) and ozone and hydrogen peroxide levels in the air. The influence of the following compounds was tested: nitrogen dioxide (NO_2), carbon monoxide (CO), volatile organic compounds (VOC), benzene, toluene and xylene (BTX). According to the model, H_2O_2 volume fractions in air increase with higher relative humidity and higher initial values of CO, VOC, BTX, H_2O_2 and O_3. Higher initial NO_2 values cause a decrease in H_2O_2 volume fractions. Ozone volume fractions in air rise with the increase of initial volume fractions of NO_2, CO, VOC, BTX, H_2O_2 and O_3. Temperature does not have any significant influence on the formation of H_2O_2 and O_3.

ProBiS: A WEB SERVER FOR DETECTION OF STRUCTURALLY SIMILAR PROTEIN BINDING SITES

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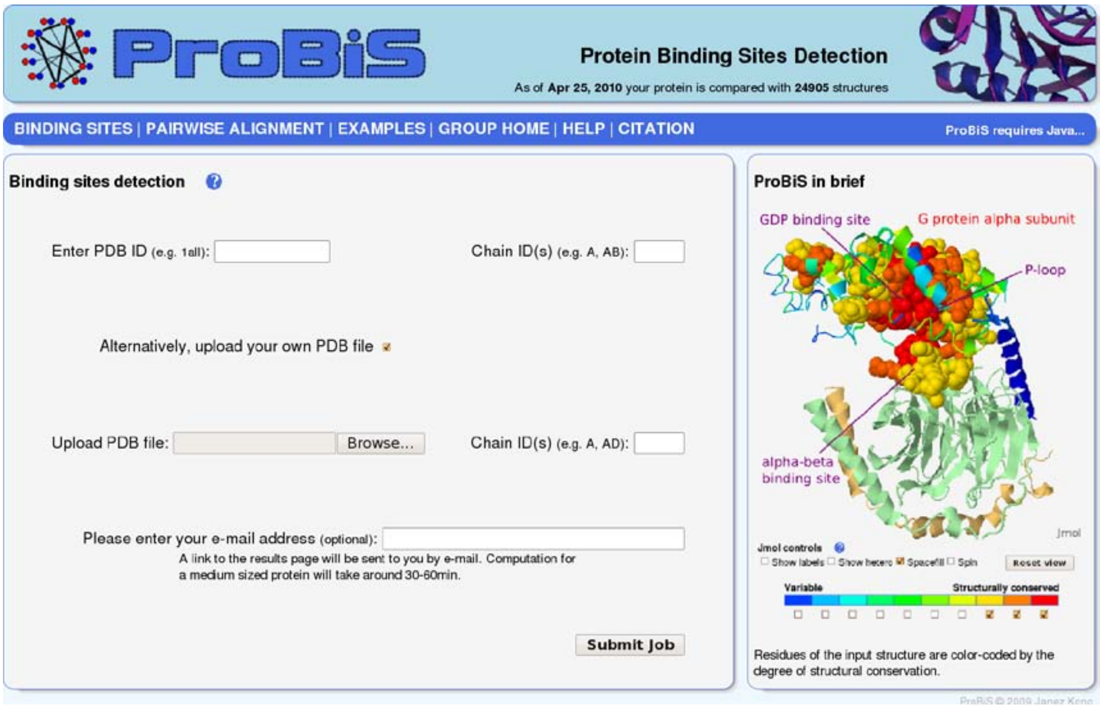
A web server, ProBiS, freely available at `http://probis.cmm.ki.si`, is presented. This provides access to the program ProBiS (Protein Binding Sites), which detects protein binding sites based on local structural alignments. Detailed instructions and user guidelines for use of ProBiS are available at the server under 'HELP' and selected examples are provided under 'EXAMPLES'.



As of Apr 25, 2010 your protein is compared with 24905 structures

A link to the results page will be sent to you by e-mail. Computation for a medium sized protein will take around 30-60min.

Residues of the input structure are color-coded by the degree of structural conservation.

THE FULLERENES – WHERE THE SCIENCES AND ARTS MEET TO MUTUAL ADVANTAGE

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The discovery of the Fullerenes, the family of closed pure–carbon cage molecules, has resulted in an elegant example of the way in which the Sciences – including Mathematics and Engineering – and the Arts – including Architecture and Design – can conflate to result in a synergistic advance which has made fascinating contributions to almost every area of intellectual interest and understanding. In recent years scientific instruments, such as microscopes and telescopes, have revealed spectacular, awe–inspiring images of the micro/nano–cosmos and the cosmos respectively. Some would argue that such images are what is called "Found Art" and thus intrinsically different from "Works of Art"! This presentation will explore these issues, using the Fullerenes as examples, to achieve a deeper, richer understanding of human creativity and enjoyment. A nice example of "Found Science" will be presented; a project whose sole motivation was the creation of an “objet d’art” and which serendipitously resulted in a major advance in our understanding of the nanoscale structure of materials and the mechanisms involved will be discussed.

GLOBAL EDUCATIONAL IN THE GOOYOUWIKI WORLD (GYWW) – THE LAST CHANCE FOR THE SURVIVAL OF AN ENLIGHTENED WORLD?

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It might be argued that, apart from some notable exceptions, the benefits of Science Engineering and Technology (SET) have generally outweighed the bad as the quality of life as well as the health of most people has improved enormously – at least in the developed world. It is not at all clear that our political leaders have the necessary wisdom to govern in a 21st Century so precariously balanced on Science, Engineering and Technology (SET). It is also clear that few members of the public have any real understanding of science, even though they are totally enveloped in an everyday environment revolutionised by the assiduous application of an evidence–based approach to what may be true. A massive improvement in the Political and Public Understanding of Science and Engineering etc (PPAUSE) will be necessary to realize both the future humanitarian promise of SET and/or impose the limitations that will safely constrain the dangers of our technologies. The recent interference by politicians in science teaching in schools should be recognised as presenting a serious threat to the future of the US. The present level of ignorance of SET is a sure recipe for disaster. Education is not that good…but it is all we have.

> *Although good decision–making cannot be guaranteed by knowledge, common sense suggests that wisdom is an unlikely consequence of ignorance.*

Some years ago I set up The Vega Science Trust to create a platform for expert scientists and engineers to communicate directly on issues that interest and/or concern them. Vega (`www.vega.org.uk`) is streaming science lectures, interviews, discussions, workshops as well as careers programs – in fact programs on a wide range of issues – all free on the Internet. 75 of the 200 programmes presently streaming were broadcast by the BBC. A new, less-expensive initiative, Global Educational Outreach for Science, Engineering and Technology (GEOSET) – has been initiated at Florida State University. It is a program that recognises the fantastic potential for shifting the paradigm of the educational process that the GooYouWiki–World (GYWW), born at the start of the 21st Century, has created. GEOSET uses a dual window format consisting of a video coupled with synchronised, downloadable, supplementary material (*e.g.*, powerpoint images, *etc*). The primary focus is the empowerment of teachers worldwide by giving them access to the very best teaching materials, packaged for their direct use in the classroom. New recording technology allows us to create effective teaching programmes and make them available globally.

> *Wherever there is a TV set, the Internet should also be able to reach and so provide teachers with the educational weapon they need to combat ignorance.*

The searchable gateway site is at `www.geoset.info` and the local site at `www.geoset.fsu.edu`.

ANALYTICAL FORMULAS FOR CALCULATING CURVATURE EFFECTS AND HYBRIDIZATION IN ZIGZAG CARBON NANOTUBES

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The electronic properties of carbon nanotubes are usually obtained with the help of the zone folding method, which is based on the graphene electronic structure. During the rolling up procedure both the angles and the inter–atomic distances are changing in the hexagonal carbon network. Thus in more sophisticated calculations curvature effects and the corresponding hybridizations must be taken into account. Usually the zone folding method is based on the simplest tight–binding (TB) approximation where each atom contains only one orbital and the off–diagonal parameter is γ_0. We call it π–tight–binding method (πTB) as the applied atomic orbital is mostly of π character.

In the all–valence tight–binding (AVTB) calculation each carbon atom is supplied by four atomic orbitals 2s, $2p_x$, $2p_y$, and $2p_z$. In the case of nanotubes with small radius one has to use at least the AVTB method or *ab initio* methods in order to take into account the hybridization effects, as for example the AVTB and the *ab initio* methods show the nanotube (5, 0) to be metallic and the zone folding πTB method predicts non–metallic character for the same tube. It was developed a modified π–tight–binding method (πTB*) using three parameters γ_1, γ_2, and γ_3 for the three first neighbour off–diagonal matrix elements of the Hamiltonian. Due to the hybridization and curvature effects, it was assumed further, that γ_i is reduced by a factor of $\cos\alpha_i$ where α_i is the angle between two nearest–neighbouring atoms. However this parameterization produced a gap for nanotube (5, 0) just like the πTB method. Here we present analytical formulas for the dispersion relations $E_\mu(\mathbf{k})$ and the γ_i parameters will be adjusted to energy values obtained by an AVTB method. In this way we shall study the possibility of substituting the AVTB calculation by a modified πTB* one.

THE RANDIĆ INDEX OF DENDRIMER NANOSTARS

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Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application. Randić index is one of them. For a graph G, the Randic index $\chi(G)$ of G is defined by:

$$\chi(G) = \sum_{i-j} \frac{1}{\sqrt{d_i d_j}}$$

with i–j ranging over all pairs of adjacent vertices of G. Dendrimers are highly branched organic macromolecules with successive layers or generations of branch units surrounding a central core. In this article, we compute the Randić index of three infinite classes of Phosphorus dendrimers, Polyphenylene dendrimers and Polymer dendrimers.

Keywords: Randić index, dendrimer nanostars

J. Hofkens, M. Maus, T. Gensch, T. Vosch, M. Cotlet, F. Köhn, A. Herrmann, K. Müllen, F.C. DeSchryver (2000) *J. Am. Chem. Soc.*, **122**: 9278–9288.

P.D. Zoon, *Single Molecule Spectroscopy with Confocal Microscopy*, `http://staff.science.uva.nl/~zoon/sms/SMS.html`

K. Yamamoto, M. Higuchi, S. Shiki, M. Tsuruta, H. Chiba (2002) *Nature*, **415**:509–511.

A.R. Ashrafi, P. Nikzad (2009) *Digest J. Nanomater. Biostruct.*, **4**:269–273.

M. Randić (1975) *J. Am. Chem. Soc.*, **97**:6609-6615.

B. Bollobás, P. Erdös (1998) *Ars Combinatoria*, **50**:225–233.

Z. Mihalić, N. Trinajstić (1992) *J. Chem. Educ.*, **69**:701–712.

D. Morales, O. Araujo (1993) *J. Math. Chem.*, **13**:95–106.

M. Randić, P.J. Hansen, P.C. Jurs (1988) *J. Chem. Inf. Compute. Sci.*, **28**:60–68.

E. Estrada (1999) *Chem. Phys. Lett.*, **312**:556–560.

E. Estrada (1995) *J. Chem. Inf. Compute. Sci.*, **35**:1022–1025.

Lj. Pavlović, I. Gutman (2001) *Novi. Sad J. Math.*, **31**:53–58.

L. Hao, M. Lu (2005) *MATCH Comm. Math. Comput. Chem.*, **54**:417–423.

K–DOMINATION SETS ON SOME SPECIAL TYPES OF 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 k–dominating set, $k \geq 1$, if for every vertex $v \in V(G) \setminus D$, there exists at least one vertex $w \in D$, such that $d(v,w) \leq k$.
The k–domination number $\gamma_k(G)$ is the cardinality of the smallest k–dominating set.
Hexagonal chains are the graph representations of an unbranched catacondensed benzenoids. Many graph invariants, which have great importance in chemistry, were investigated on these types of graphs. Some of them are Hosoya index, Merrifield–Simmons index and eigenvalues of adjacency matrix. Interesting results were obtained and it has been shown that there are three species of hexagonal chains which are extremal due to above topological invariants. These are the linear chain L_h, helicene chain H_h and zig–zag chain Z_h.
k–domination number, as another interesting graph invariant, was already studied on L_h.
In this paper we present k–dominating sets on H_h and Z_h and we determine upper bound for $\gamma_k(H_h)$ and $\gamma_k(Z_h)$.

NMR CONFORMATIONAL STUDIES AND MOLECULAR MODELING OF NOVEL BIS–PORPHYRIN SUPRAMOLECULAR SYSTEMS

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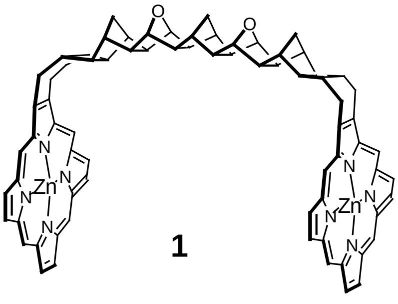
Here we report NMR conformational studies and computational modeling of a novel bis–porphyrin supramolecular system **1** designed for use in photovoltaic devices. Variable temperature ^{1}H–NMR spectroscopy (both at high and at low temperatures) was employed, and in conjuction with 2D COSY and NOESY experiments used for structural assignments and to determine conformational behaviour of system **1**. In addition, semiempirical quantum–chemical (AM1) and density functional (B3LYP) calculations were conducted. The combined results of this study indicate that **1** exists in dynamic equilibrium, in which porphyrin rings can flip around cyclohexene ring from etended to U–shaped structure. However, the equilibrium favors the U–shaped structure shown in Fig. 1.



1

Figure 1.

REALITY OF THE ZERO POINT ENERGIES?

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The Einstein's cosmological constant is often associated with the Casimir effect, proving thus reality of the zero point energies of quantum fields. However, Casimir effects and Casimir forces can be obtained without reference to zero point energies (R.L. Jaffe, 2005). We report here a similar result obtained for a quantum scalar field in an external classical scalar field. We also calculated the corresponding probability distribution of the zero point energy density.

MOLECULAR VIBRATIONS: ACCOUNT ON VIBRATIONAL WAVEFUNCTIONS AND POTENTIAL ENERGY SURFACES

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In this course we review several concepts linked to molecular vibrations. First we examine the Born–Oppenheimer approximation and define the nuclear Schrodinger equation. Within this framework we survey the harmonic approximation and introduce normal–mode analysis. A modal–based approach is subsequently used to define both the potential energy surface (PES) and the nuclear Hamiltonian. This provides the machinery to go beyond harmonic approximation and gives the key to understand vibrational structure theory. On one side, few modal–based methods for the construction of the PES are analyzed, putting special emphasis on current methods used for vibrational calculations. Besides, a few methods to solve the nuclear Schrodinger equation are examined. The connection between the level of approximation chosen for both the PES and the vibrational wavefunction is throughout studied.

EIGENVALUES FOR SOME PARTICULAR GRAPHS

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The matrices attached to molecular graphs represent a large source of topological invariants useful in analysis of quantitative structure – properties relationship.[1] The eigenvalues of these matrices (the graph spectra) and especially the largest eigenvalues are also useful for theoretical studies of graphs.[2]

The paper describes the variation of the largest eigenvalues of adjacency (A), distance (D) and Laplacian (La) matrices for some well known graphs (path, star, complete connected graphs) but also for some particular graphs like trees with branches with equal number of vertices on each branch, trees with constant growing of vertices on each branch (spiral like trees) and spider–silk graphs (Fig. 1a and 1b, respectively).

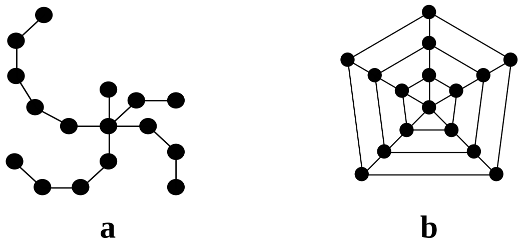

Figure 1: Spiral like graphs and spider–silk like graphs

This paper also describes how to setup higher order Laplacian matrices and the variation of their largest eigenvalues.

J. Devillers, A.T. Balaban (Eds.) (1999) *Topological Indices and Related Descriptors in QSAR and QSPR,* Gordon and Breach, Amsterdam.

D. Cvetković, P. Rowlinson (1990) The Largest Eigenvalue of a Graph: A Survey*, Lin. Multilin. Algebra*, **28**:3-33.

THE MODIFIED WIENER INDEX OF NANOSTRUCTURES

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Suppose G is a graph, $u \in V = V(G)$, $A \leq \mathrm{Aut}(G)$ and $g \in \mathrm{Aut}(G)$. Define $d(u,V) = \sum_{x\in V} d(u, x)$, $\delta(g) = \frac{1}{|V|}\sum_{u\in V} d(u, g(u))$, $\delta(A) = \frac{1}{|A|}\sum_{g\in A} \delta(g)$, and $\delta(G) = \delta(\mathrm{Aut}(G))$.

The notion of modified Wiener index, $\overline{W}(G)$, was introduced by Graovac and Pisanski (1991). It is defined as $\overline{W}(G) = \frac{1}{2}|V(G)|^2\ \delta(G)$.

In this talk, some formulae for computing modified Wiener index of some nanotubes, nanotori and nanostars are presented.

Keywords: modified Wiener index, nanotube, nanotorus, nanostar dendrimer

A. Graovac, T. Pisanski (1991) On the Wiener index of a graph, *J. Math. Chem.*, **8**:53–62.
S. Yousefi, H. Yousefi–Azari, A.R. Ashrafi, M.H. Khalifeh (2008) Computing Wiener and Szeged indices of a polyhex nanotorus, *J. Sci. Univ. Tehran*, **33**(3):7–11.

THE ECCENTRIC POLYNOMIALS OF SOME NEW CLASS OF NANOSTRUCTURES

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Carbon nanotubes are allotropes of carbon with a cylindrical nanostructure. These cylindrical carbon molecules have novel properties that make them potentially useful in many applications in nanotechnology, electronics, optics and other fields of materials science. The eccentric connectivity polynomial $\Xi(G, x)$ is defined as:

$$\Xi(G, x) = \sum_{u \in V(G)} \deg(u)\, x^{\varepsilon(u)},$$

where deg(u) denotes the degree of vertex u and $\varepsilon(u)$ is the largest distance between u and any other vertex of G.[1–3]

In this talk, we present our latest results in computing formulas for the eccentric connectivity polynomials of some new type of nanostructures.

1. V. Sharma, R. Goswami, A.K. Madan (1997) Eccentric connectivity index; A novel highly discriminating topological descriptor for structure property and structure activity studies, *J. Chem. Inf. Comput. Sci.*, **37**:273–282.
2. A.R. Ashrafi, T. Došlić, M. Saheli (2011) The eccentric connectivity index of $TUC_4C_8(R)$ nanotubes, *MATCH Commun. Math. Comput. Chem.*, **65**, in press.
3. V. Kumar, S. Sardana, A.K. Madan (2004) Predicting anti–HIV activity of 2,3–diaryl–1,3–thiazolidin–4–ones: Computational approach using reformed eccentric connectivity index, *J. Mol. Model.*, **10**:399–407.

COMPUTING TWO TYPES OF GEOMETRIC–ARITHMETIC INDEX OF TUC$_4$C$_8$(S) NANOTUBE

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Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Recently a class of so called geometric–arithmetic (GA) topological indices is defined as the sum over all edges (uv) of a (molecular) graph G, of term

$$\frac{\sqrt{Q_u Q_v}}{\frac{1}{2}(Q_u + Q_v)},$$

where Q_u is quantity associated with the vertex u of G.

One invariant of GA was obtained for Q_u being the number n_u of vertices of G lying closer to vertex u than to v. This type of GA index is defined by:

$$GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u n_v}}{\frac{1}{2}(n_u + n_v)}.$$

Another one was obtained for the number m_u of edges of G lying closer to vertex u than to vertex v, and is defined by:

$$GA_3(G) = \sum_{uv \in E(G)} \frac{\sqrt{m_u m_v}}{\frac{1}{2}(m_u + m_v)}.$$

In this paper GA$_2$ and GA$_3$ indices of TUC$_4$C$_8$(S) nanotube is computed.

G. Fath–Tabar, B. Furtula, I. Gutman (2010) A new geometric–arithmetic index, *J. Math. Chem.*, **47**:477–486.

M. Ghorbani, M. Jalali (2009) Computing a new topological index of nano structures, *Dig. J. Nanomater. Bios.*, **4**:681–685.

Y. Yuan, B. Zhou, N. Trinajstić (2010) On geometric–arithmetic index, *J. Math. Chem.*, **47**:833–841.

B. Zhou, I. Gutman, B. Furtula, Z. Du (2009) On two types of geometric–arithmetic index, *Chem.Phys. Lett.*, **482**:153–155.

EXTREMAL POLYOMINO CHAINS WITH RESPECT TO THE ECCENTRIC CONNECTIVITY INDEX

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Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The eccentric connectivity index $\xi(G)$ of a graph G is defined as:

$$\xi(G) = \sum_{u \in V(G)} \deg(u)\, \varepsilon_G(u),$$

where $deg(u)$ denotes the degree of vertex u in G and $\varepsilon_G(u)$ is its eccentricity.

A polyomino system is a finite 2–connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. In other word, it is an edge–connected union of cells in planar square lattice.

In this paper, the explicit formula of eccentric connectivity index of linear chain and zig–zag chain is given, and the extremal polyomino chains with respect to the eccentric connectivity index are determined.

T. Došlić, A. Graovac, O. Ori (2010) Eccentric connectivity indices of hexagonal belts and chains, *submitted*.
T. Došlić, M. Saheli, D. Vukičević (2010) Eccentric connectivity index: Extremal graphs and values, *submitted*.
M.J. Morgan, S. Mulwembi, H. C. Swart (2010) On the eccentric connectivity index of a graph, *Discrete Math.*, in press.
L. Xu, S. Chen (2008) The PI index of polyomino chains, *Appl. Math. Lett.*, **21**:101–1104.
B. Zhou, Z. Du (2010) On eccentric connectivity index, *MATCH Commun. Math. Comput. Chem.*, **63**:181–198.

A NOVEL METHOD FOR COMPUTING EDGE WIENER INDEX OF DENDRIMER NANOSTARS

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Let G be a connected graph and $\psi(G) = Sz_e(G) - W_e(G)$ where $W_e(G)$ denotes the edge Wiener index and $Sz_e(G)$ denotes the edge Szeged index of G. In an earlier paper, it is proved that if T is a tree then $Sz_e(T) = W_e(T)$. In this paper, we continue our work to prove that for every connected graph G, $Sz_e(G) \geq W_e(G)$ with equality if and only if G is a tree. A new classification for the graphs with $\psi(G) = 1, 2, 3, 4, 5$ are also presented. Finally, we prove that for each non–negative integer n, there exists a graph G with $\psi(G) = n$. We apply this method to compute the edge Wiener index of some classes of dendrimer nanostars.

Keywords: edge Szeged index, edge Wiener index, dendrimer nanostar

I. Gutman, A.R. Ashrafi (2008) The edge version of the Szeged index, *Croat. Chem. Acta*, **81**(2):263–266.

M.H. Khalifeh, H. Yousefi–Azari, A.R. Ashrafi, S. Wagner (2009) Some new results on distance–based graph invariants, *Eur. J. Combin.*, **30**(5):1149–1163.

TOPOLOGICAL SYMMETRY OF DENDRIMERS

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Dendrimers are one of the main objects of nanobiotechnology. They possess a well defined molecular topology. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this talk, the mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of these macromolecules. We prove that it is possible to write the symmetry group of a dendrimer, as wreath product of some finite groups. To prove, we consider two infinite classes of dendrimers and compute their topological symmetry groups.

Keywords: symmetry group, dendrimer, wreath product

A.R. Ashrafi (2005) *MATCH Commun. Math. Comput. Chem.*, **53**:161–174.
A.R. Ashrafi (2005) *Chem. Phys. Lett.*, **403**:75–80.
The GAP Team, GAP–Groups (1995) *Algorithms and Programming, Lehrstuhl D für Mathematik, RWTH*, Aachen.

MOLECULAR OVALITY DESCRIPTORS IN MODELING THE TOXICITY OF ALIPHATIC ESTERS ON TETRAHYMENA PYRIFORMIS

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Quantitative structure–activity relationships (QSARs) were developed for a series of alcohols which exhibit toxic activity, A, to the ciliate protozoan Tetrahymena pyriformis. A = log(1/IGC$_{50}$), where IGC$_{50}$ represents the 50% inhibiting growth concentration. The molecular descriptors used in this paper, Θ_{iD}, D = 1,2,3, were constructed on the basis of the molecular van der Waals (vdW) space, considered homogeneous, isotropic, and compressible in some extent. Θ_{1D} and Θ_{3D} shape descriptors are, respectively, one–dimensional and two–dimensional extensions of the Θ_{2D} molecular shape parameter defined as the ratio of molecular surface area over surface area of a sphere with identical volume. The QSAR analysis was performed by means of the MobyDigs software. The quality and the robustness of the all–three linear models A *vs.* Θ_{iD} were analyzed and the corresponding values of the statistics were evaluated and reported here. The slightly better results were obtained for Θ_{iD} ovality descriptor:

$r^2 = 0.830,\ r^2_{adj} = 0.826,\ q^2_{LOO} = 0.814.$

The predictive power is good, taking into account the commonly accepted values for a satisfactory QSAR model: $q^2 > 0.500$. It has been shown in this study that accurately describing the toxicity of aliphatic esters with a single correlation is quite feasible if the molecular descriptors have clear physical meaning, and they are related to the physical and chemical interacting forces between molecules, and particularly between biological receptors of biological membranes and the toxin molecules.

THE ROLE OF PATH INTEGRALS IN QUANTUM CHEMISTRY

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Aiming in providing a dynamical physical, mathematical, and computational integrated framework for solving the chemical structure and reactivity of many–electronic systems, the path integral formalism is approached at both fundamental and applicative levels. The lecture is envisaged to cover the following basic and advanced items:

- From density matrix to path integral. Application on electronic densities;
- Feynman's path integral of evolution amplitude. Harmonic oscillator;
- Semiclassical path integral evolution amplitude. Application on periodic system of chemical reactivity indices of electronegativity and chemical hardness;
- Effective classical path integral of evolution amplitude. Feynman–Kleinert variational formalism. Stability of matter. Connection with Density Functional Theory (DFT). Absolute electronegativity scale by Feynman centroid;
- Non–equilibrium path integral of evolution amplitude. Application on Markovian processes. Connection with Electronic Localization Functions (Markovian–ELFs).

R.P. Feynman (1948) *Rev. Mod. Phys.*, **20**:367–387.
R.P. Feynman, H. Kleinert (1986). *Phys. Rev.* A, **34**:5080–5084.
H. Kleinert, A. Pelster, M.V. Putz (2002) *Phys. Rev.* E, **65**(6):066128/1–7.
M.V. Putz, N. Russo, E. Sicilia (2005) *Theor. Chem. Acc.*, **114**(1–3):38–45.
M.V. Putz (2005) *Int. J. Quantum Chem.*, **105**(1):1–11.
M.V. Putz (2007) *J. Theor. Comput. Chem.*, **6**(1):33–47.
M.V. Putz (2008) *Absolute and Chemical Electronegativity and Hardness*, Nova Publishers Inc., N.Y.
M.V. Putz (2009) *Int. J. Mol. Sci.*, **10**(11):4816–4940.

THE PI–INDEX OF SOME NANO STRUCTURES

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Let G be a simple connected graph. If $e = uv$ is an edge of G and $m_u(e)$ is the number of edges closer to u than v and $m_v(e)$ is the number of edges closer to v than to u then the PI (Padmakar–Ivan) and Sz_e (Szeged) indices of G are defined as:
$PI(G) = \Sigma_{e=uv}\, m_u(e) + m_v(e)$
and
$Sz_e(G) = \Sigma_{e=uv}\, m_u(e)\, m_v(e)$.
In this paper, the PI, Szeged and GA_2 (geometric–arithmetic) indices of two types of dendrimers are computed for the first time.

Keywords: PI index, edge Szeged index, nanostar dendrimer

G.H. Fath–Tabar, A.R. Ashrafi, I. Gutman (2009) Note on Estrada and L–Estrada indices of graphs, *Bull. Acad. Serbe Sci. Arts Cl. Sci. Math. Natur.*, **139**:1–16.

G.H. Fath–Tabar, M.J. Nadjafi–Arani, M. Mogharrab, A.R. Ashrafi (2010) Some inequalities for Szeged–like topological indices of graphs, *MATCH Commun. Math. Comput. Chem.*, **63**:145–150.

SOME OLD PROBLEMS AND SOME NEW RESULTS REVISITED

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As graduate student over 50 years ago in Cambridge (England) I attended a fascinating lecture of Linus Pauling which started with structure of H_2O and ended with a picture of a tail of bacteriophage (any one of a number of viruses that infect bacteria). In this lecture I will attempt to review selected old and new problems related to application of Graph Theory to molecules – wide but much more modest goal that nevertheless will cover some of my interests over the past 50 years. I will briefly revisit HMO and point to its overlooked potentials and I will end with novel matrices in chemistry, including novel distance matrix, matrices that count amino acids adjacency, frequency of separations of the same amino acids in proteins, and latest characterizations of proteomics maps using partial ordering of amino acids with respect to their charges and masses, and using Voronoi diagrams.

title to be announced

Milan RANDIĆ, Dejan PLAVŠIĆ

ESTIMATION OF THE OVERALL STABILITY CONSTANT OF CADMIUM(II) BIS–COMPLEXES WITH ALIPHATIC α–AMINO ACIDS USING $^3\chi^v$ INDEX

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For the estimation of the overall stability constant, β_2:

$$\mathrm{M + L + A} \overset{\beta_2}{\rightleftarrows} \mathrm{MLA} \qquad (1)$$

where M denotes Cd^{2+} and L and A denote α–amino acids, we developed regression function:

$$\log \beta_2 = a_1[^3\chi^v(\mathrm{MLA})] + a_2[^3\chi^v(\mathrm{ML})] + a_3[\,^3\chi^v(\mathrm{MA})/\,^3\chi^v(\mathrm{ML})] + b \qquad (2)$$

assuming $^3\chi^v(\mathrm{ML}) \leq {}^3\chi^v(\mathrm{MA})$.

The model was tested on measured 14 binary and ternary (mixed) cadmium(II) *bis*–complexes with five aliphatic α–amino acids (glycine, alanine, and 2–aminobutanoic, 2–aminopentanoic, and 2–aminohexanoic acid), with the range of $\log \beta_2^{\mathrm{exp}} = 6.88 – 7.47$.[1] Log β_2 values were reproduced fairly well with errors = 0.02 – 0.19 and $S.E._{cv} = 0.10$, which is close to the errors of other models for the estimation of stability constants of coordination compounds.[2]

1. H. Matsui, H. Ohtaki (1982) *Bull. Chem. Soc. Jpn.*, **55**:461–465, 2131–2133.
2. N. Raos, A. Miličević (2009) *Arh. Hig. Rada Toksikol.*, **60**:123–128.

DENSITY FUNCTIONAL B3LYP AND B3PW91 STUDIES OF THE PROPERTIES OF SOME CYCLIC ORGANODIBORANES

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Cyclic organodiboranes with a unique stable intramolecular doubly hydrogen–bridged structure, such as 1,2–tetramethylenediborane and 1,2:1,2–bis(tetramethylene)diborane, have been the subject of some debate. Molecular structure and vibrational spectra of 1,2–tetramethylene diborane(I),1,2:1,2–bis (tetramethylene) diborane(II), 1,1–tetramethylenediborane(III) and 1,1:2,2–bis(tetramethylene) diborane (IV), have been studied employing quantum computational density functional B3LYP and B3PW91 methods using 6–31G*, 6–31G** and 6–31++G** basis sets. Results of the structural investigation showed that all of these alkyldiboranes have non–planar structures. In I and III alkyldiboranes the B–H$_{(t)}$ bonds are shorter than the B–H$_{(b)}$ bonds, which is indicative of reduction bond order in B–H$_{(b)}$ bonds. The vibrational analysis was carried out on the optimized structures in the B3LYP and B3PW91 method by using 6–31++G** basis set. The results characterize that all of the optimized structures have minima on the potential energy surface without any negative mode. The obtained results showed that B–H$_{(t)}$ stretching band is rather than the B–H$_{(b)}$ adsorption band and verify the bond of the B–H$_{(t)}$ is shorter than the B–H$_{(b)}$. The population analysis showed that there are significant cross populations between indirectly bonded B–B atoms of the ring at the two DFT methods for the alkyldiborane with six–member ring (I). The NBO analysis demonstrated the strain present in the alkyldiborane rings, attributable largely to the ~sp^{2} hybridization of the boron atom. However, the possibility must also be considered that the excess stability of the double hydrogen bridge of compounds I and III, as evidenced by its relatively low reactivity toward terminal olefins, may also be playing an important role in the ease of the ring opening reaction with diborane.

GLOBAL FORCING NUMBER OF THE BENZENOID PARALLELOGRAM

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A global forcing set in a simple connected graph G with a perfect matching is any subset S of $E(G)$ such that the restriction of the characteristic function of perfect matchings of G on S is an injection. The number of edges in a global forcing set of the smallest cardinality is called the global forcing number of G. We prove that for benzenoid parallelogram with m rows and n columns of hexagons ($m \leq n$) global forcing number equals

$$\frac{m(n+1)}{2}$$

if m is even, and

$$\frac{n(m+1)}{2}$$

if m is odd.

Also, we provide an example of global forcing set with smallest cardinality.

THEORETICAL STUDY OF HYDROGEN ADSORPTION AND DIFFUSION IN SPILLOVER PROCESS ON MICROPOROUS CARBON

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Using path integral simulation with density functional theory (DFT) calculation, we investigated the hydrogen distribution on microporous carbon such as zeolite templated carbon (ZTC).[1,2] Evaluation of chemisorption energies of a hydrogen atom on four graphene–like fragments with different curvature (Fig. 1) showed that hydrogen atoms adsorb strongly at the edge site and convex surface. We also showed that hydrogen chemisorption at edge sites enhances the adsorption energy at the inner site.

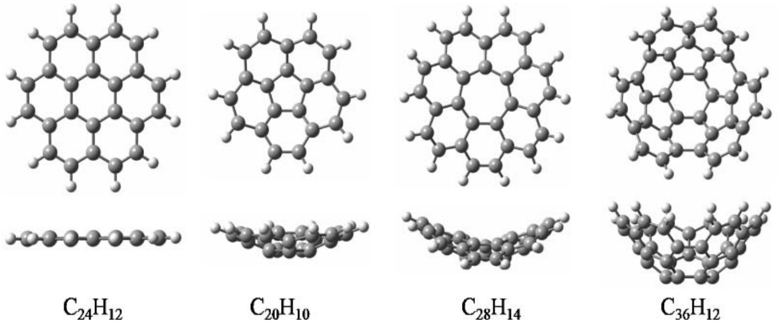

Figure 1. Front and side views of molecular structures of $C_{24}H_{12}$ (coronene, [6]circlene), $C_{20}H_{10}$ (corannulene, [5]circlene), $C_{28}H_{10}$ (pleiadannulene, [7]circlene), and $C_{36}H_{12}$ (triacenaphthotriphenylene).

To reveal the mechanism of hydrogen diffusion on a carbon surface in the spillover process, transition states of two types were examined: hydrogen moving along the C–C bond keeping a weak C–H bond, and hydrogen dissociation from the carbon surface. The results suggest that the latter path is more likely to occur than the former path in flat surface and the situation might be modified by introducing curvature.

These results suggest that efficiency of hydrogen spillover on carbon–based hydrogen storage materials will be enhanced by controlling the structure of the carbon surfaces.

This work was conducted as a collaborative effort between the New Energy and Industrial Technology Development Organization (NEDO) projects "Advanced Fundamental Research on Hydrogen Storage Materials (Hydro-Star)" and “Development of Technologies for Hydrogen Production, Delivery and Storage Systems”.

1. H. Nishihara, P.–X. Hou, L. –X. Li, M. Ito, M. Uchiyama, T. Kaburagi, A. Ikura, J. Katamura, T. Kawarada, K. Mizuuchi, T. Kyotani (2009) *J. Phys. Chem.* C, **113**: 3189–3196.
2. H. Nishihara, Q. –H. Yang, P. –X. Hou, M. Unno, S. Yamauchi, R. Saito, J.I. Paredes, A. Martínez–Alonso, J.M.D. Tascón, Y. Sato, M. Terauchi, T. Kyotani (2009) *Carbon*, **47**:1220–1230.

INTRINSIC FORMULA FOR FIVE POINT ATIYAH DETERMINANTS

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In 2001 Sir M. F. Atiyah formulated a conjecture C1 and later with P. Sutcliffe two stronger conjectures C2 and C3. These conjectures, inspired by physics (spin–statistics theorem of quantum mechanics), are geometrically defined for any configuration of points in the Euclidean three space. The conjecture C1 is proved for n = 3, 4 and for general n only for some special configurations (M.F. Atiyah, M. Eastwood and P. Norbury, D. Đoković). In a lengthy preprint[1] we have verified the conjectures C2 and C3 for parallelograms, cyclic quadrilaterals and some infinite families of tetrahedra. We have also proposed a strengthening of the conjecture C3 for configurations of four points (Four Points Conjectures) and a number of conjectures for almost collinear configurations.

Eastwood and Norbury[3] found an intrinsic formula for the four point Atiyah determinant (a polynomial of sixth degree in six distances having several hundreds of terms) and gave a proof of C1. The present author found a new geometric fact for arbitrary tetrahedra and a proof of C2 and C3 for arbitrary four points in three space.

The main aim of the talk is to give a formula in the title which may lead to a proof of five point Atiyah conjectures (with a more powerfull computers !). So far we get a polynomial formula (for five points) and have an existence proof of a polynomial formula for all planar configurations what was conjectured.[2]

Our proof produces also trigonometric formulas for Atiyah determinants (not known before even for four points).

1. D. Svrtan, I. Urbiha, Verification and Strengthening of the Atiyah–Sutcliffe Conjectures for Several Types of Configurations, arXiv: math/0609174 (49 pages).
2. M. Eastwood, P. Norbury (2001) A Proof of Atiyah's Conjecture on Configurations of Four Points in Euclidean Three Space, *Geom. Topol.*, **5**: 885–893.
3. M. Atiyah, P. Sutcliffe (2002) The Geometry of Point Particles. arXiv: hep–th/0105179 (32 pages*). Proc. R. Soc. Lond.* A, **458**:1089–1115.
4. M. Atiyah, P. Sutcliffe (2003) Polyhedra in Physics, Chemistry and Geometry, arXiv: math–ph/03030701 (22 pages), *Milan J. Math*., **71**:33–58.
5. D. Svrtan, I. Urbiha, Atiyah–Sutcliffe Conjectures for almost Collinear Configurations and Some New Conjectures for Symmetric Functions, arXiv: math/0406386 (23 pages).
6. M. Atiyah, An Unsolved Problem in Elementary Geometry, `www.math.missouri.edu/archive/Miller-Lectures/atiyah/atiyah.html`
7. M. Atiyah, An Unsolved Problem in Elementary Euclidean Geometry, `http//c2.glocos.org/index.php/pedronunes/atiyah-uminho`

THEORETICAL STUDY ON THE GROUND AND EXCITED STATES OF 3,5–DIACETYL–1,4–DIHYDROLUTIDINE

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The *ab initio* molecular orbital calculations are performed on the lutidine derivatives (3,5–diacetyl–1,4–dihydrolutidine, IUPAC name 3,5–diacetyl–1,4–dihydro–2,6–dimethylpyridine (DL1) and its substitutions, 3,5–dibenzoyl–1,4–dihydro–2,6–dimethylpyridine (DL2) and 3,5–dibenzoyl–1,4–dihydro–2,6–diphenylpyridine (DL3)). These compounds have absorption peaks around 410 nm, which is used for the detection of formaldehyde by the acetylaceton method in aqueous solution.

The electronic structures of the ground and excited states of DL1 are studied using *ab initio* molecular orbital method at the HF/3–21G, CIS/3–21G, B3LYP/6–31G(d,p) and TD B3LYP/6–31G(d,p) levels., and that of the ground states of DL2 and DL3 are studied at the HF/3–21G and B3LYP/6–31G(d,p) levels.

The optimized structure of the ground and first excited state of DL1 shows the C=C and C=O bond lengths become shorter with a one electron excitation from HOMO to LUMO, whereas the C-C and C-N bond lengths become shorter.

The S_0-S_1 transition energy of DL1 is calculated to be 372 nm which slightly overestimates the experimental absorption spectrum 410 nm, and the S_1-S_0 transition energy of DL1 is calculated to be 435 nm which also overestimates the experimental value 510 nm.

As a model of DL1 in the aqueous solution and the porous glass, we also calculate the electronic structures of complexes of DL1 with an H_2O and an $H_2Si{=}O$. The LUMO of the $H_2Si{=}O$ complex is that of $H_2Si{=}O$, whereas the LUMO of the H_2O complex is that of DL1. As a result, H_2O molecule does not affect on the low–lying excited states of DL1, however, the low–lying excited state of the $H_2Si{=}O$ complex contain the contribution from the $H_2Si{=}O$ moiety and would have a slightly different natures from DL1. This fact would be attributed to an unexpected stability of the lutidine derivatives (DL1–DL3) in the porous glass.

PREDICTION ACCURACY MAY NOT PROVE HYPOTHESIS: THE CYSTEINE–CYSTINE CASE

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Predictive potential is considered to be the best proof of a hypotheses. Therefore one can expect that prediction methods based on certain hypotheses and not on artificial intelligence have two kinds of profit. Beside the practical use of an accurate prediction method, these can prove the principle on which the prediction method is based. Here we present an example that it is not always true: prediction accuracy may not prove the basic hypothesis of a prediction method. We show that while the oxidation state of residue Cys can be predicted from the information on the local sequence environment of these residues, most of the information about the oxidation state is not stored in this local sequence. Instead, this local sequence, similarly to the sequence information of any polypeptide segment of similar size determines the subcellular location of the protein analyzed and this location is the one which primarily determines the oxidation state of residue Cys in question.

CaGe – A VIRTUAL ENVIRONMENT FOR STUDYING SOME SPECIAL CLASSES OF PLANE GRAPHS

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CaGe (Chemical and Abstract Graph Environment) is an environment for generating and visualizing certain specialized classes of plane graphs with the emphasis on classes that are relevant in chemistry.

A first version of CaGe was described in Ref. 1 and since then CaGe was used by various researchers for much varying purposes (see Refs. 2, 3, 4, for example applications). The first version of CaGe was based on Tcl/Tk, but due to several problems with the speed and the development of Tcl/Tk, we decided that instead of repeatedly updating CaGe, we should better develop and support a new version based on Java. This Java based version was first released in 2001 and since then continuously updated (see Ref. 5 for the Changes History).

Compared to the version described in Ref. 1 the new version offers various new features and generators for more classes of graphs. Furthermore it is more portable now and runs under Unix/GNU–Linux and Mac OS X. Currently the development of CaGe is based in both Bielefeld and Ghent. Last year a major reworking of the code and the interface of CaGe was done: we made the interface which had grown organically during the years more uniform. At the same time we documented the code to allow for easier maintenance and extension.

A session with CaGe basically works as follows. You start by making a first coarse selection, followed by a refinement step. Next you set the parameters for the generator. Once these parameters have been set, CaGe will determine which generator to use. Mostly there is just one choice but for some cases (*e.g.* cubic graphs with given faces) there are multiple possibilities and the generator that is expected to be the most efficient one is chosen. The final step before the generator is started is to specify the output. CaGe has the option to first pipe the results of the generator through a filter program which may add extra restrictions on the graphs that weren't implemented in the original generator. The graphs can be drawn in 2 and 3 dimensions, an adjacency matrix can be given and even an unfolding of the 3 dimensional structure can be outputted. Any combination of these options is also possible. Currently CaGe has 3 embedders: one general embedder which uses different techniques and is described in Ref. 6, and two specialized embedders for nanocones and nanotubes. Once the generator is running you can browse through the results using the navigation window.

1. G. Brinkmann, O. Delgado Friedrichs, A. Dress, T. Harmuth (1997) CaGe – a virtual environment for studying some special classes of large molecules, *MATCH Commun. Math. Comput. Chem.*, **36**:233–237.
2. S. Schein, T. Friedrich (2008) A geometric constraint, the head–to–tail exclusion rule, may be the basis for the isolated–pentagon rule in fullerenes with more than 60 vertices, *Proc. Natl. Acad. Sci. USA*, **105**(49):19142–19147.
3. H. Zettergren, G. Sanchez, S. Diaz–Tendero, M. Alcami, F. Martin (2007) Theoretical study of the stability of multiply charged c–70 fullerenes. *J. Chem. Phys.*, **127**, article number: 104308.
4. P.W. Fowler, P. Hansen, D. Stevanović (2003) A note on the smallest eigenvalue of fullerenes, *MATCH Commun. Math. Comput. Chem.*, **48**:37–48.
5. Homepages of CaGe: `http://www.mathematik.uni-bielefeld.de/~CaGe` and `http://caagt.ugent.be/CaGe`.
6. O. Delgado Friedrichs (2006) Fast embeddings for planar molecular graphs, in: P. Hansen, P. Fowler, M. Zheng (Eds.) *Discrete Mathematical Chemistry* Vol. **51** of DIMACS Series in Discrete Mathematics and Theoretical Computer Science, American Mathematical Society, pp. 85–95.
7. G. Brinkmann, O. Delgado Friedrichs, S. Lisken, A. Peeters, N. Van Cleemput (2010) CaGe – a Virtual Environment for Studying Some Special Classes of Plane Graphs – an Update, *MATCH Commun. Math. Comput. Chem.*, **63**:533–552.

BOND ADDITIVE MODELING – RANDOMNESS *vs.* DESIGN

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Predictions of properties of octane isomers proposed by International Academy of Mathematical Chemistry (IAMC) will be analyzed. Recently it was shown that one–parameter linear models based on the Adriatic descriptors have higher correlation coefficient *r* for 10 out of 16 properties than the analogous models based on the benchmark set of descriptors proposed by IAMC. However, it is possible that some of these results are the results of the pure chance. Here, we propose the series of five additional tests to test whether these results are obtained by chance or if they are the result of insightful design. It is indicated that the predictions of the melting point (not even analyzed[1]), density (results commented as doubtful[1]), molar volume (also results commented as doubtful[1]), heat capacity and octanol–water partition coefficient at *P* constant may be the results of pure chance and it seems that predictions of heat capacity at *T* constant, enthalpy of vaporization, standard enthalpy of vaporization, molar octane number and total surface area are the results of the insightful design.

1. D. Vukičević, M. Gašperov, Bond Additive Modeling 1. Adriatic Indices, *Croat. Chem. Acta*, accepted for publication.

STRUCTURE ANALYSIS AND HUB DETECTION IN COMPLEX NETWORKS

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We present a structural analysis of complex networks. More specifically, we speak about communities and hubs in the networks.

We examine Estrada’s method for community structure detection and some of its properties.

We additionally propose a novel method for fast detection of hubs within a system. The algorithm identifies a set of nodes in the network as most significant, aimed to be the most effective points of distribution for fast, widespread coverage throughout the system. We show that our hubs have in general greater closeness centrality and betweenness centrality than vertices with maximal degree, and have in general higher degree than vertices with greatest closeness centrality and betweenness centrality. As such, they serve as all–purpose network hubs. Several theoretical and real world networks are tested and results are analyzed.

We further develop a classification of three types of hubs related to the spread of SIR–type epidemics. We define a network outhub as a node which, if infected first, causes the most extensive spread of a disease throughout the network. An inhub is a node which is most likely to become infected at some point during the spread of the disease through the system. And a network transitive hub is a node which, if vaccinated, most decreases the spread of the disease through the system. We show that on some networks, these three hubs are distinct, indicating the need for more specific identification of network hubs than the general use of vertex degree and connectivity.

COMPUTING THE FIRST GEOMETRIC–ARITHMETIC INDEX OF SOME NANO STRUCTURES

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Investigations of topological indices based on end–vertex degrees of edges have been conducted over 35 years. One of them is the first geometric–arithmetic index (GA_1). The GA_1 index defined as:

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)},$$

has been introduced less that a year ago (Vukičević & Furtula, 2009).

In this paper the first geometric–arithmetic index is computed for some nanotubes, nanotorus and nanostars.

D. Vukičević, B. Furtula (2009) Topological index based on the ratios of geometrical and arithmetical means of end–vertex degree of edges, *J. Math. Chem.*, **46**:1368–1376.

M. Ghorbani, M. Jalali (2009) Computing a new topological index of nano structures, *Dig. J. Nanomater. Bios.*, **4**:681–685.

THE ECCENTRIC CONNECTIVITY INDEX OF AN INFINITE FAMILY OF NANOSTAR DENDRIMERS

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Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For two vertices u and v of $V(G)$ we define their distance $d_G(u, v)$ as the length of the shortest path connecting u and v in G. For a given vertex u of $V(G)$ its eccentricity $\varepsilon G(u)$ is the largest distance between u and any other vertex v of G. Hence

$$\varepsilon_G(u) = \max_{v \in V(G)} d_G(u,v).$$

The eccentric connectivity index $\xi(G)$ of a graph G is defined as:

$$\xi(G) = \sum_{u \in V(G)} \deg(u)\, \varepsilon_G(u),$$

where $deg(u)$ denotes the degree of vertex u in G and $\varepsilon_G(u)$ is its eccentricity.

The nanostar dendrimers belong to a new group of macromolecules that act as photon funnels and artificial antennas and show a great resistance to photo bleaching. Experimental and theoretical insight is needed in order to understand energy transfer mechanism in these macromolecules. In recent year, some researchers studied mathematical properties of these nanostructures. In this paper, the eccentric connectivity indices of an infinite family of nanostar dendrimers are computed.

T. Došlić, M. Saheli, D. Vukičević (2010) Eccentric connectivity index: Extremal graphs and values, *submitted*.
T. Došlić, A. Graovac, O. Ori (2010) Eccentric connectivity indices of hexagonal belts and chains, *submitted*.
A. Ilić, I. Gutman (2010) Calculating the eccentric connectivity index of chemical trees, *MATCH Commun. Math. Comput. Chem.*, in press.

THE BIPARTITE EDGE FRUSTRATION OF AN INFINITE FAMILY OF FULLERENES

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Let $G = (V, E)$ be a simple graph. A spanning subgraph is a subgraph that contains all the vertices of original graph. The *bipartite edge frustration* of G, denoted by $\varphi(G)$, is the smallest number of edges that have to be deleted from a graph to obtain a bipartite spanning subgraph. It is easy to see that (G) is a topological index and G is bipartite if and only if $\varphi(G) = 0$. Thus $\varphi(G)$ is a measure of bipartivity. It is well–known fact that a graph G is bipartite if and only if G does not have odd cycles. Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make fullerene graph bipartite. In this paper we compute the bipartite edge frustration of an infinite family of fullerene graphs.

T. Došlić, D. Vukičević (2007) Computing the bipartite edge frustration of fullerene graphs, *Discrete Appl. Math.*, **155**: 1294–1301.

M. Ghojavand, A.R. Ashrafi (2008) Computing the bipartite edge frustration of some nanotubes, *Dig. J. Nanomater. Bios.*, **3**:209–214.

Z. Yarahmadi, T. Došlić, A.R. Ashrafi, The bipartite edge frustration of composite graphs, *Discrete Appl. Math.*, in press.

WIENER INDEX OF DENDRIMER NANOSTARS

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Suppose G is a graph and $d_G(x, y)$ denotes the length of a minimum path connecting vertices x and y of G. A *distance–based topological index* is a topological index related to the distance function d_G. The Wiener index $W(G)$ is the first distance–based topological index introduced by Wiener for investigating boiling point of alkanes.[1] This index is defined as the sum of all distances between vertices of the graph under consideration (see Refs. 2 and 3 for details). The definition of the Wiener index in terms of distances between vertices of a graph was first given by Hosoya.[4]
In our presentation, we report the latest results in computing Wiener index of dendrimer nanostars.

1. H. Wiener (1947) Structural determination of paraffin boiling points, *J. Am. Chem. Soc*., **69**:7–20.
2. A.A. Dobrynin (1998) Discriminating power of the Schultz index for catacondensed benzenoid graphs, *MATCH Commun. Math. Comput. Chem.,* **38**:19–32.
3. A.A. Dobrynin, R. Entringer, I. Gutman (2010) Wiener index of trees: Theory and applications, *Acta Appl. Math.*, **66**:211–249.
4. H. Hosoya (1971) Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *B. Chem. Soc. Jpn.*, **44**:2332-2339.