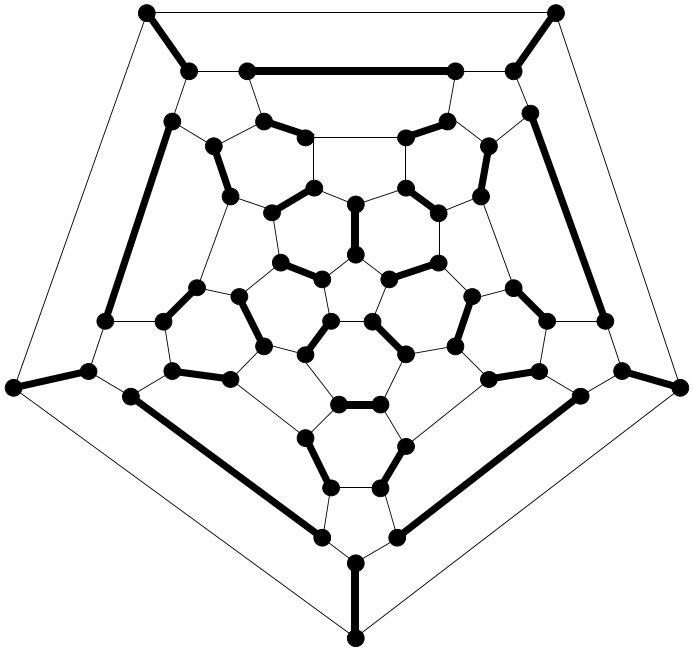
Book of Abstracts

Visualization and Modeling in Chemistry



Bilateral Croatian-Slovenian Conference

Split, Croatia

October, 29-31, 2010.

Visualization and Modeling in Chemistry

Bilateral Croatian-Slovenian Conference

Dedicated to Professor Ante Graovac in happy celebration of his 65th birthday

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Editor

Damir Vukičević

Contents

Foreword

Conference *Visualization and Modeling in Chemistry* is bilateral Croatian-Slovenian Conference. The financial support of the Croatian Ministry of Science Technology and Sports and Slovenian Ministry of Higher Education, Science and Technology is gratefully acknowledged. Conference participation is per invitation only and all lectures are invited lectures.

We are very glad that one of the pioneers and leading figures of chemical graph theory and great friend to all participants of this conference, Professor Ante Graovac, is our guest of honor. We dedicate this conference to him in happy celebration of his 65^{th} birthday.

The development of new fields of chemistry demands interdisciplinary research and the main goal of this conference is to combine experimental work and mathematical modeling in order to solve selected problems in various fields of chemistry. Several different topics will be discussed, that is, creation and visualization of atmospheric reaction schemes, modeling of chemical fate of toxic organic compounds and modeling of biologically active compounds. Developments in the research of chemical descriptors will be presented as well as the analyses of their discriminativity, predictivity and extremal properties. One of goals is also to expand the collaboration of graph-theorists on the reliability of the visualization problems. New algorithms and/or improvements and applications of the existing algorithms for visualization problems are to be presented. The most important purpose of this conference is to gather a critical mass of scientists that could be able to submit a sound proposal for the joint projects funded by the European Union. Other conference goals are:

1) Strengthening the collaboration between mathematicians and chemists on development of new scientific results in mathematical chemistry;
2) collaboration of graph-theorists on the reliability and visualization problems;
3) collaboration of algorithm theory experts, mathematicians and bio-informaticians in furthering knowledge in bio-informatics;
4) meeting of Croatian and Slovenian experts in atmospheric chemistry;
5) collaboration of experts in algorithm theory and atmospheric chemistry on the development of algorithms in atmospheric chemistry.

Proceedings of this conference will be included in the special issue of the journal *International Journal of Chemical Modeling* dedicated to Professor Graovac.

It is a great pleasure to welcome you and whish you fruitful and enjoyable conference.

Dear Professor Graovac, happy birthday and let all your good wishes come true!

Organizers:
Damir Vukičević, director
Matevž Pompe, co-director
Tanja Vojković, co-director

Conference Program

Friday, October 29, 2010

14:00-16:00 Registration and welcome drink

16:00-16:40 Opening ceremony

Nanostructures and conjugated hydrocarbons (chair: Damir Vukičević)

16:40-17:10 Ante Graovac: *Topological Coordinates for Carbon Nanostructures*

17:10-17:40 Milan Randić: *Graph Theoretical Approach to π-Electron Currents in Polycyclic Conjugated Hydrocarbons*

17:40-18:10 Mircea V. Diudea: *All-Pentagonal Face Nano-Dendrimer and Related Structures*

18:10-18:40 COFFEE BREAK

Peptides and Proteins (chair: Milan Randić)

18:40-19:10 Mirjana Novič: *Visualization of Protein Sequences and Classification of Trans-membrane Segments*

19:10-19:40 Davor Juretić: *Structural asymmetries and biological activity of membrane-transforming-peptides*

20:00- DINNER

Saturday, October 29, 2010

08:00-09:00 BREAKFAST

Molecular Descriptors I (chair: Matevž Pompe)

09:00-09:30 Damir Vukičević: *Bond Additive Modeling*

09:30-10:00 Janez Žerovnik: *Graphs with given number of cut-edges and minimal value of Szeged and Revised Szeged index*

10:00-10:30 Tomislav Došlić: *Augmented eccentric connectivity index*

10:30-11:00 COFFEE BREAK

Molecular Descriptors II (chair: Ante Graovac)

11:00-11:30 Ivan Gutman: *The Graph-Energy Desease*

11:30-12:00 Nenad Trinajstić: *On Sum-Connectivity Index, a Novel Addition to the Family of Connectivity Indices*

12:00-12:30 BREAK

Molecular Descriptors III (chair: Tomislav Došlić)

12:30-13:00 Lorentz Jäntschi: *Distribution of QSARs correlation coefficients*

13:00-13:30 Martin Šala: *QSAR model for the estimation of toxicological effects of organic chlorinated pollutants*

13:30- LUNCH

Air Pollution (chair: Martin Šala)

17:30-18:00 Matevž Pompe: *Calibration of mass selective detector in non-target analysis of volatile organic compounds in the air*

18:00-18:30 Leo Klasinc: *Photochemical pollution indicators from ozone data*

18:30-19:00 COFFEE BREAK

Researching with(in) EU (chair: Dragutin Svrtan)

19:30-20:00 Boris Horvat: *Researching with(in) EU*

20:00- DINNER

Sunday, October 29, 2010

08:00-09:00 BREAKFAST

Mathematics (chair: Janez Žerovnik)

09:00-09:30 Dragutin Svrtan: *New Brahmagupta formula and its applications to intrinsic geometry of cyclic polygons*

09:30-10:00 Primož Lukšić: *NP-hardness of the distance-balanced edge addition problem*

10:00-10:30 COFFEE BREAK

Applications (chair: Boris Horvat)

10:30-11:00 Iztok Kavkler: *Visual method for measurement of flow velocity*

11:00-11:30 Veljko Zlatić: *New materials for thermoelectric applications: theory and experiment*

11:30-11:45 Closing Ceremony

12:00- LUNCH

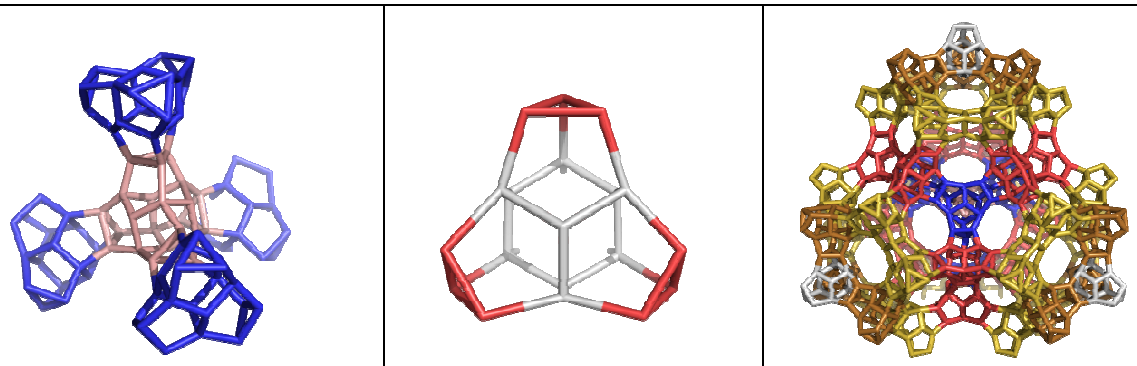
All-pentagonal face nano-Dendrimer and related Structures

Mircea V. Diudea

"Babeş-Bolyai" University Cluj-Napoca, Cluj, Romania

Abstract

A nano-dendrimer built up by a monomeric unit, made by all-pentagonal polyhedral faces, is used in a (self-assembly) growing process to provide either a dendrimer or a multi toroidal nano-structure Figure). It is shown that the monomer and some small intermediates, as hydrogenated species, have a moderate stability, between adamantane and C_{60} fullerene. The topology of these nanostructures is described in terms of Omega polynomial, function of the net parameters.[1-5] Close formulas for this polynomial and examples are tabulated.



M_5; v=98	M_1; v=22; e=36; f_5=12; g=2	4S_MT; v=972

Figure. A nano-dendrimer at 1st generation (left) and its core (central); it becomes a multi torus, at 5th generation

Keywords: nano-dendrimer; multi torus; Omega polynomial.

Acknowledgments:

This paper is dedicated to Professor Ante Graovac on the occasion of his 65th birthday.

Thanks to organizers and Mediterranean Institute for Life Sciences for covering the expanses at conference site.

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Augmented eccentric connectivity index

Tomislav Došlić

Faculty of Civil Engineering, University of Zagreb, Croatia

The augmented eccentric connectivity index has been much used recently in the QSAR/QSPR studies. In spite of its usefulness, its mathematical properties have never been properly investigated. The main goal of this presentation is to review some basic mathematical properties of the augmented eccentric connectivity index and, where possible, to establish explicit formulas for certain classes of graphs. It turns out that those properties are very far from the properties of other distance-based invariants such as, e.g., the Wiener number and the eccentric connectivity index. We find that this is due to the combined effects of the non-local and non-linear nature of the vertex contributions. We also point out several unsolved problems and list some possible directions for future research.

Topological Coordinates for Carbon Nanostructures

Ante Graovac[1, 2]

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[2]*The R. Boskovic Institute, POB 180, HR-10002 Zagreb, Croatia*

The topological coordinates method is an effective approach to generate good initial Cartesian coordinates for fullerenes, nanotubes and toroidal carbon structures using only the connectivity graph of a given structure. Usually they are obtained by diagonalization of the adjacency matrix of the molecular graph and are based on the so called bi-lobal eigenvectors. For spherical surfaces as fullerenes three bi-lobal eigenvectors are sufficient but the topological coordinates of tori are constructed with the help of four bilobal eigenvectors. We supposed firstly that the nanotubes junctions made of three finite nanotubes are homeomorphic to the sphere and used three bi-lobal eigenvectors to derive their topological coordinatees but some problems appeared which have been then removed when we turned to the eigenvectors of the corresponding Laplacean matrices. However, the choice of eigenvectors and their appropriate combinations to get plausible geometries of junctions is a subtle procedure.

This work and related shape analysis of nanostructures were done in collaboration with Professors István László of Budapest, Hungary, and Tomaž Pisanski of Ljubljana, Slovenia.

The Graph-Energy Desease

Ivan Gutman

Faculty of Science, University of Kragujevac, Kragujevac, Serbia

The energy of a graph is equal to the sum of the absolute values of the eigenvalues of the adjacency matrix. The graph-energy concept was put forward in 1978, although its chemical roots go be to the 1940s. Research on graph energy became quite popular in mathematics and mathematical chemistry, resulting in hundreds of papers (and hundreds of results) in the last 10-15 years.

The analogue of graph energy, based on the eigenvalues of the Laplacian matrix (the "Laplacian energy") was introduced in 2006, followed by the energy based on the edigenvalues of the distance matrix (the "distance enerrgy") in 2008. In 2007 Nikiforov showed how the energy-concept can be extended to arbitrary matrices, including non-square matrices.

In recent years we are faced with a flood of new "graph energies". We mention here (in alphabetical order): α-distance energy, α-incidence energy, energy of (0,1)-matrices, Harary energy, incidence energy, Laplacian-energy like invariant, normalized Laplacian energy, Randić energy, signless Laplacian energy, skew energy, sum-connectivuty energy, Szeged energy, Todeschini-type descriptors, ...

We will show that some of these "energies" are mutually related, sometimes in a mathematically non-trivial manner. However, most of the papers in which the new "energies" are being introduced and studied, contain only elementary and straighforward consequences of the proposed definition, and redundant results, usually lower and upper bounds.

The lecturer, who is one of the initiators and culprits, is now looking for some means to stop the spreading of the desease.

Researching with(in) EU

Boris Horvat

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Various kinds of EU regulated project funding is available through different calls. While providing additional funding for research & development activities at Universities and Institutes, the organization and bureaucracy involved in applying, managing and reporting represent new additional knowledge, requiring team organization and development of certain managing and administrative skills, in addition to core research activities. It is of utmost importance for public research organizations to organize adequately in order to be capable to obtain such types of funding.

As Croatia is going to become a member of EU in near future, new types of project calls are available for contribution of Croatian institutions. As EU member, in Slovenia we already have some experience with projects of that type, which also include national projects funded by European Social Fund and European Regional Development Funds.

Large majority of such project calls are not strictly focused to research but more to development (of any kind), and hence including applied research and development. However, various calls may support applications of various projects where involvement of mathematics and computer science depends on creativity and proactivity of related institutions forming consortia and developing the content. One such call is IPA (Instrument of Pre accession Assistance), which is a mechanism for support of cooperation with EU candidate countries. Other such call was InterReg, which was directed to cross-border cooperation. Research related calls in majority go through FP7 programme. A kind of hybrid calls (EU + local) which are directed specifically to research are calls by European Science Foundation ESF. We shall present our experience in organizing consortium and applying for ESF's call EuroGiga (project Gregas) and SI-CRO IPA call (project TESHUB), as well as experience from carrying out several projects financed by European Social Fund or European Regional Development Fund.

Distribution of QSARs correlation coefficients

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[b] *"Iuliu Haţieganu" Medicine and Pharmacy University of Cluj-Napoca, Cluj, Romania*

[c] *"Babeş-Bolyai" University Cluj-Napoca, Cluj, Romania*

[d] *Agricultural Sciences and Veterinary Medicine Cluj-Napoca, Cluj, Romania*

Abstract

A set of ordnance compounds, with size ranging from 5 (one case) to 8 (11 cases) was previously studied about the effect in aquatic environment (on the marine life). For a number of 24 biological activities, at which a computed property was added (OPLS-SAE), a pool of simple linear regressions relating the activity and structure by using the MDFV methodology (implying creation of a pool of descriptors and addressing of adaptation criteria to the descriptors) was developed. From the pool of simple linear regressions the ones being statistically significant (probability to reject the linear model less or equal to 0.05) were selected. A study regarding the distribution of the correlation coefficients for the selected simple linear regressions was performed. Three distribution laws were proved to be relevant for the population of correlation coefficients (Beta, Generalized Pareto and Pert). For these three distributions a further study regarding the classification of the activities into one or another distribution was made. The study has shown that the Chi-Square statistic was the best classifier of the activities: only one disagreement with the true positive classification of simultaneously independent events of all three. The outcome of the study is that 48% of the correlation coefficients populations of significant simple linear regressions are Beta distributed, 40% are Generalized Pareto, and the rest - 12% - including the OPLS-SAE, are Pert distributed.

Keywords: *Structure-Activity Relationships; Distribution laws; Correlation coefficients*

Acknowledgments:

This paper is dedicated to Professor Ante Graovac on the occasion of his 65th birthday.

Thanks to organizers and Mediterranean Institute for Life Sciences for covering the expanses at conference site.

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Structural asymmetries and biological activity of membrane-transforming-peptides

Davor Juretić[1]

[1]*Department of Physics, Faculty of Science, University of Split, Split, Croatia*

Membranes have multifunctional and vital roles in all living cells. Less recognized fact is that membranes are mainly composed of amphipathic lipids with asymmetric distribution between outer and inner membrane leaflets, which is significantly different for cytoplasmic membrane of Gram-positive bacteria, Gram-negative bacteria, mammalian and cancer cells. Fusogenic peptides, cell-penetrating peptides and antimicrobial peptides are all the subject of intensive research during last 25 years as membrane-active peptides, due to potential applications in medicine, health care, food production and preservation, but published results describing how their structure and mechanism of action are connected with biological activity are often speculative and even contradictory. Taking amphipathic helical peptides as a common example, different types of helical peptides are usually classified according to biological activity, which can differ for several orders of magnitudes, even when their mean physicochemical properties are similar. It is likely that helical peptides may exhibit very different mechanisms of perturbing and restructuring biological membranes, depending on membrane type, peptide sequence and ionic strength of a solution. For the example of anuran antimicrobial peptides acting on Gram-negative bacteria and human red blood cells, we shall see that structural asymmetries in peptide primary structure can distinguish those with hemolytic properties, those with selective activity as mediocre peptide antibiotics and those with selective activity as excellent peptide antibiotics. Visualization tools should be able to see similar asymmetries in peptide 3D structure, but peptide backbone structure is certainly not enough for the job. We shall explore in this work how structural asymmetries due to residue type, sequence position and orientation in peptide helical structure may be connected to membrane-transforming and biological activity.

Visual method for measurement of flow velocity

Iztok Kavkler[1], Alen Orbanić[1], Brane Sirokz[2], Matjaž Eberlinc[2], Tom Bajcar[2]

[1]*Institute of Mathematics, Physics and Mechanics, Jadranska 19, 1000 Ljubljana, Slovenia*

[3]*University of Ljubljana, Faculty of Mechanical Engineering, Aškrčeva 6, 1000 Ljubljana, Slovenia*

There are several methods for measuring velocities of fluid or gas flows. Most of them are very expensive since they require an elaborate setup of sensors immersed into the flow. Moreover, these methods are impractical for certain types of liquids, e.g. liquid metal, where the use of sensors is impossible. A much cheaper method is to apply some pollutant and track it visually using a camera. Due to the two-dimensional nature of visualization, these methods works best when the flow is naturally restricted to two dimensions.Our implementation differs from some others that use pattern recognition to reconstruct flow velocity. Instead, we measure the local density of the pollutant and calculate flow velocity via diffusion-advection equation. The problem is in general ill-posed, therefore we need extra techniques to obtain best possible results.

Photochemical pollution indicators from ozone data

Tomislav Cvitaš[1], Nenad Kezele[2], Leo Klasinc[2],
Elvira Kovač-Andrić[3], Glenda Šorgo[2]

[1]Department of Chemistry, University of Zagreb,Zagreb,
[2]Rudjer Bošković Institute,Bijenička 54, Zagreb
[3]Department of Chemistry, J.J. Strossmayer University of Osijek, Osijek

We have recently (see: Photochemical pollution indicators – an analysis of 12 European monitoring stations. *Environmental Monitoring and Assessment*, **165** (2010) 577-583) developed new indicators that can be used to analyse photochemical pollution and smog caused by ozone. The indicators are based on simple mathematical formulae and could make it easier for those who monitor pollution levels to make meaningful comparisons between different sites. The approach has been selected for inclusion in Science for Environment Policy the European Commission's environmental news service for policy makers, distributed to over 11,000 subscribers on 8/07/10 .See:

http://ec.europa.eu/environment/integration/research/newsalert/archive/air_pollution_10.htm

We will report results that are based upon early ozone measurements in Zagreb and cities along the Adriatic coast and some islands from before 1990.

NP-hardness of the distance-balanced edge addition problem

Primož Luksić,

UL FMF & IMFM, Slovenija

It a graph has the sum of the distances from a chosen vertex to all other vertices equal for all the vertices, it is called a self-median graph. Connected self-median graphs are also distance-balanced (and vice-versa), which are known in mathematical chemistry. For example, bipartite distance-balanced graphs have the maximal Szeged index among all graphs of the same size, while distance-balanced graphs have the maximal revised Szeged index.
We consider the following optimization problem: given a graph, add the minimum possible number of edges to obtain a distance-balanced graph. We show that the problem is NP-hard for graphs of diameter three. In contrast, we show that the problem can be solved in polynomial time for graphs of diameter 2.

The presentation is prepared in the colaboration with Sergio Cabello.

Visualization of Protein Sequences and Classification of Trans-membrane Segments

Amrita Roy Choudhury, Marjana Novič

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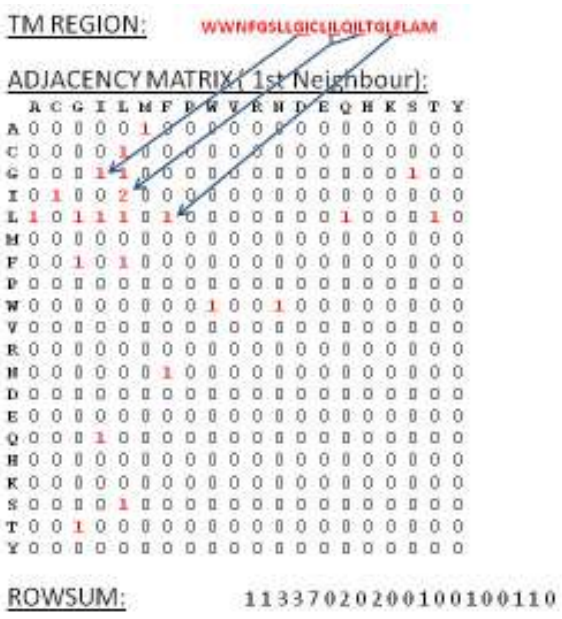
Majority of membrane transport proteins of known sequences are not yet resolved for their 3D structure, which is of great importance in the study of the protein transport mechanism. The method presented here exploits the information about the structure of trans-membrane segments of proteins of known 3D structure available in public databases. The constructed model is able to predict the trans-membrane domains of structurally unresolved target protein within 10% error for alpha helices[1], while the prediction of beta shaped trans-membrane segments is less accurate and is still being improved. With the help of known structures the trans-membrane domains are encoded using discrete mathematics[2] in such a way that it is possible to group and classify them with respect to their specific sub-structural characteristics and to build a model for prediction of trans-membrane segments. The model was interpreted and tested on bilitranslocase, the transporter of organic anions from blood to liver cells.



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Calibration of mass selective detector in non-target analysis of volatile organic compounds in the air

Gregor Arh[1], Leo Klasinc[2], Marjan Veber[1], Matevž Pompe[1]

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Volatile organic compounds (VOC) play an important role in the chemistry of the atmosphere and in biogeochemistry. They contribute to the oxidative capacity of the atmosphere, particle and air pollutants, as well as to the production of greenhouse gasses (for instance ozone). Among analytical techniques for their determination in the atmosphere gas chromatography coupled with mass spectrometry (GC-MS) offers several advantages. However, for an accurate quantification calibration with standard substances is necessary. A quantitative structure-property relationship (QSPR) model for the prediction of MS response factors was developed on basis of our experimental measurements for the quantification of ozone precursors present in the atmosphere. A linear correlation between chemical structures and response factors was established by using a partial least-square model. The error in the prediction of response factors was calculated by cross-validation procedure and was below 20%, which is sufficient for the determination of VOCs in the air.

Graph Theoretical Approach to π-Electron Currents in Polycyclic Conjugated Hydrocarbons

Milan Randić

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New Brahmagupta formula and its applications to intrinsic geometry of cyclic polygons

Dragutin Svrtan

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Finding formulas for the area (or circumradius) of polygons inscribed in a circle ,with given side lengths, is a classical subject. The famous Heron's and Brahmagupta's formulas give the answer for triangles and cyclic quadrilaterals. Only in 1994. D.P.Robbins found a minimal equation for the area of cyclic pentagons and hexagons, by using the undetermined coefficient method. Even reproving directly these formulas ,by using elimination theory, was quite a challenge due to complexity of symbolic computations. With a new Brahmagupta's formula we succeded in finding an intrinsic proof (with an intriguing elimination procedure) . For cyclic heptagons the undetermined coefficient method was hardly applicable (143307 equations) and M.F. Maley, D.P.Robbins and J.Roskies (in 2004) produced (by using covariants of binary quintic) a formula in the form of a quotient of two resultants,which we have recently expanded to a polynomial with 955641 terms having coefficients up to 40 digits (a 5000 pages formula). For the area times circumradius equations we obtained ,by a similar method ,an explicit formula with 31590 terms having coefficients up to 11 digits. With the help of our new Brahmagupta formula we get minimal area equation for cyclic heptagons/octagons, in all concrete instances considered so far (we conjecture for all), by using Groebner basis for a system of only three equations.So far we are not able to do symbolic Groebner basis computations –computers are still to slow to do this. By a different method (Wiener Hopf factorization) we get a minimal circumradius equation for cyclic heptagons/octagons in a condensed (Pellian) form with up to 4 digits coefficients (a 15 pages formula).These formulas may be of some use in computing volumes of fullerens.

QSAR model for the estimation of toxicological effects of organic chlorinated pollutants

Martin Šala, Alexandru T. Balaban, Marjan Veber, Matevž Pompe

Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, 1000 Ljubljana, Slovenia,

In order to perform the screening of new potential pollution points and to estimate their impact on the environment, a quantitative structure-activity research (QSAR) modeling procedure was used to estimate possible toxicological effects of the substances that were introduced into the environment due to modifications of traditional food products (TFP) production processes. We have focused our study initially to known persistent toxins with defined toxicological mechanisms. Such groups of studied chemicals were polychlorinated aromatic compounds.

Three parttial least-square (PLS) models were developed for the calculation of aryl hydrocarbon receptor (AhR) binding affinity of chlorinated biphenyls, dibenzofurans and dioxins. In all cases models were able to explain more than 70% of the total variance. Additionally, an encoding capability of the newly developed variable Balaban's distance topological index was tested. It showed reasonable modeling abilities but superior interpretation abilities compared to classical PLS QSAR models.

On Sum-Connectivity Index, a Novel Addition to the Family of Connectivity Indices*

Bono Lučić,[1a] Jadranko Batista,[2] Sonja Nikolić,[1b] Dražen Vikić-Topić,[1a]

Dejan Plavšić,[1a] Nenad Trinajstić[1b]

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In 1975, Randić proposed a structural descriptor that has become a well-known molecular descriptor called the connectivity index.[1-3] This descriptor found a considerable use in QSPR and QSAR.[4-6] The connectivity index χ is defined as[1]

$$\chi(G) = \sum_{uv \in E(G)} \left(d_u d_v\right)^{-1/2},$$

where G denotes molecular graph, d_u is the degree (valency) of vertex u and $E(G)$ is the edge-set of G. For convenience $\chi(G)$ is called the product-connectivity index. There are a number of variants of product-connectivity index available in the literature,[1-6] but no one considered *sum* instead of *product* of the vertex-degrees in the above expression. A novel connectivity index ${}^{s}\chi$, called the sum-connectivity index, is defined as[7-9]

$${}^{s}\chi(G) = \sum_{uv \in E(G)} \left(d_u + d_v\right)^{-1/2}$$

Properties and some applications of this novel descriptor will be presented as well as comparison with the original connectivity index.

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*Dedicated to Professor Dr. Ante Graovac on occasion of his 65th birthday

Bond Additive modeling

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Bond additive descriptors are descriptors which value is calculated as the sum of bond contributions. In many cases these bond contributions depend solely on the bond incident degree. Such indices are called bond incident degree indices. Some of them are very well known indices, e.g. Randić index, Zagreb index, modified Zagreb index, variable Randić index, atom-bond connectivity index.

In this lecture we shall present a large class of such indices named Adriatic indices, we shall illustrate their application in the QSAR/QSPR research. A lot of open problems that may attract the attention of researchers in this area will be mentioned.

Also, in this lecture we shall present the series of mathematical tools for the study of bond incident degree indices will be presented. These tools may provide a simple way to obtain the extremal results for newly defined Adriatic indices and other bond incident degree indices that may be defined in the future.

New materials for thermoelectric applications: theory and experiment.

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I will review the current development in the field of thermoelectric and thermomagnetic energy conversion. I will discuss new materials and examine mechanisms that could lead to new thermoelectric devices with an enhanced figure-of-merit. Our main concern is an understanding of the heat and charge transport in strongly correlated systems, and our final objective is to acquire the basic knowledge about the relevant quantum degrees of freedom, which is required to achieve the control and engineer new thermoelectric and magneto-caloric materials with specific quantum mechanical properties.

Thermoelectric devices are heat engines that either convert heat into electricity or use the electricity to pump the heat from a cold to hot reservoir. The possibilities arising from the fact that electricity can be generated directly from heat, the Seebeck effect known since 1821, are beginning to be more widely appreciated. This is due to current environmental concerns to reduce waste heat loss and to find new, sustainable energy sources. The thermoelectric devices can reduce the petrol consumption in motor vehicles by 5 to 10%, reducing significantly the oil needs. They are also used for power generation in remote regions, where the thermoelectricity ensures a continuous power supply of electronic equipment. This is an important, but only one type of applications of a thermoelectric effect. The other thermoelectric effects, the Peltier effect and Thompson effect, can be used for cooling without moving parts, providing microcooling for the electronics industry and refrigeration without the use of environmentally damaging CFCs and FCs. All of these can play an important role in development and efficient use of sustainable energy resources. The scientific and technological advances in this field could have important implication for the modern society.

The main problem in nearly all of these applications is the rather low efficiency of the processes of energy conversion. The important factor which determines the efficiency is the dimensionless ratio, ZT, known as the figure of merit. This needs to be optimized to give a value of ZT of the order of 1 or higher for the more widespread use of thermoelectric devices. A value of ZT of the order 1 requires use of a material with a large thermopower and electrical conductivity and a low thermal conductivity. These tend to be incompatible requirements; for example, a good metal has a high electrical conductivity but also a high thermal conductivity. Materials which have a high thermopower tend also to have a low electrical conductivity. The aim of this research field, therefore, is to find or fabricate materials with the properties so as to enhance ZT. It is a multidisciplinary field, requiring the expertise of material physicists, chemists, metallurgists and the support of theory. There have been important recent developments in innovative synthesis techniques, the discovery of new materials, and a deeper understanding of the parameters that affect the performance materials in thermoelectric devices. These have brought the goal of producing materials with the required characteristics for commercial application a significant step closer. The aim of mz lecture is to review these exciting developments

Graphs with given number of cut-edges and minimal value of Szeged and Revised Szeged index

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Let $G_{n,k}$ denote the set of graphs with n vertices and k cut edges. Operation C on graphs is considered that is a generalization of both operations A and B studied by Hua [H.Hua, MATCH Commun. Math. Comput. Chem. 61 (2009) 643.]. It is shown that the result of operation C always reduces the values of the Szeged index and of the Revised Szeged index (also called Modified Szeged index). This observation enables identification of graphs in $G_{n,k}$ with minimal value of the Szeged index. Properties of graphs in $G_{n,k}$ with minimal value of Revised Szeged index are discussed.

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