

## A NEW METHOD FOR COMPUTING PI AND SZEGED INDICES OF EXTENDED BRIDGE GRAPH AND ITS APPLICATION IN NANOSTRUCTURES

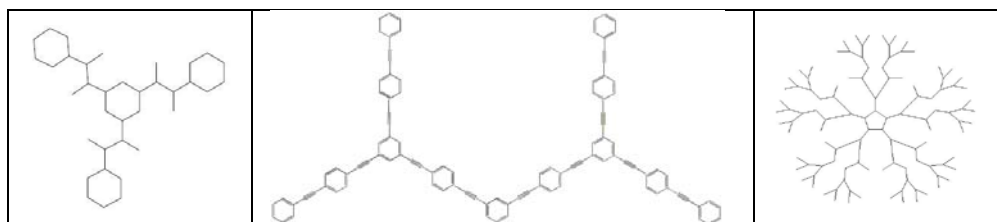
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Let  $\{H_i\}_{i=1}^n$  be a set of finite pairwise disjoint graphs with  $v_i \in V(H_i)$ . The extended bridge graph  $EB(G, H_1, H_2, \dots, H_n) = EB(G, H_1, H_2, \dots, H_n; v_1, v_2, \dots, v_n)$  of  $\{H_i\}_{i=1}^n$  with respect to the vertices  $\{v_i\}_{i=1}^n$  is constructed by identifying the vertex  $v_i$  in  $G$  and  $H_i$  and by connecting the vertices  $v_i$  and  $v_{i+1}$  by an edge for all  $i \in N$  and  $i \bmod n$ .

Here we compute the Padmakar–Ivan (PI) and Szeged indices for extended bridge graphs shown below.



## AN ALGORITHM FOR COMPUTING SOME TOPOLOGICAL INDICES BASED ON DISTANCE

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A topological index is a single unique number (graph invariant) characteristic of a molecular graph. For a simple connected graph  $G$  with vertex set  $V(G)$  and edge set  $E(G)$ , the distance between vertices  $u$  and  $v$  is denoted by  $d(u, v)$  and the maximum distance between vertices is denoted by  $d(G)$ . The Wiener index of  $G$  is defined as:

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

The Reverse Wiener index of  $G$  is defined by Balaban as:

$$RW(G) = \frac{1}{2} n(n-1)d(G) - W(G)$$

The number of steps an algorithm requires to solve a specific problem is known as the running time of the algorithm. The time complexity  $T(n)$  is a function of the problem size  $n$  and its value is the running time of the algorithm in the worst case, *i.e.*, the number of steps it requires at most with an arbitrary input. The time complexity of an algorithm is commonly expressed using big O notation which suppresses multiplicative constants and lower order terms.

In this paper we give an algorithm for computing the Wiener and Reverse Wiener indices of a connected graph. By using this algorithm and GAP program,  $W$  and  $RW$  indices for a family of fullerenes have been computed. The input of the program are adjacent vertices of each vertex and the time complexity of the program is  $O(n^4)$ .

## **DISTANCE–BASED TOPOLOGICAL INDICES OF FULLERENES**

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A mapping taking graphs as arguments is called a graph invariant or topological index if it assigns equal values to isomorphic graphs. A distance–based topological index is a topological index related to natural distance function  $d(-,-)$  on the vertex set of the graph under consideration. A fullerene molecule  $C_n$  is a closed–cage carbon molecule with three–coordinated carbon atoms tiling the spherical or nearly spherical surface with 12 pentagonal and  $n/2 - 10$  hexagonal rings. In this talk, our recent results on computing some distance–based topological indices of fullerenes are reported.

*Keywords:* fullerene, distance–based topological index

## COMPUTATION OF TWO TOPOLOGICAL INDICES AND THEIR CORRESPONDING POLYNOMIALS FOR SOME GRAPH OPERATIONS

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Let  $G$  be a simple, undirected, connected and finite graph with the set of vertices  $V(G)$  and the set of edges  $E(G)$ . Here, we denote by  $d(u, v|G)$  the distance between two vertices  $u$  and  $v$  of  $G$ . A topological index of  $G$  is a real number assigned to  $G$  and is invariant under all graph isomorphisms.

Wiener index of  $G$  is the first topological index introduced in chemistry<sup>1</sup>:

$$W(G) = \sum_{\{u,v\} \in V(G)} d(u, v|G),$$

and Wiener polynomial of  $G$  was introduced in terms of a parameter  $q$ <sup>2</sup>:

$$W(G; q) = \sum_{\{u,v\} \in V(G)} q^{d(u,v|G)}.$$

It is clear that the first derivative of the Wiener polynomial of  $G$  in  $q = 1$  is equal to the Wiener index of  $G$ .

After the Wiener index and Wiener polynomial a series of related indices and polynomials have been defined and some of them have found applications in both chemistry and mathematics.

Following this trend we defined two new indices of a graph  $G$ <sup>3</sup>:

$$Max(G) = \sum_{u \in V(G)} \sum_{[a,b] \in E(G)} \max\{d(u, a|G), d(u, b|G)\}$$

$$Min(G) = \sum_{u \in V(G)} \sum_{[a,b] \in E(G)} \min\{d(u, a|G), d(u, b|G)\}$$

and we introduced two related polynomials in terms of a parameter  $q$ <sup>4</sup>:

$$Max(G; q) = \sum_{u \in V(G)} \sum_{[a,b] \in E(G)} q^{\max\{d(u,a|G), d(u,b|G)\}}$$

$$Min(G; q) = \sum_{u \in V(G)} \sum_{[a,b] \in E(G)} q^{\min\{d(u,a|G), d(u,b|G)\}}.$$

In the second sums in the above expressions the summations go over edges of  $E(G)$ .

These two polynomials have interesting properties. For example, the first derivatives of these polynomials at  $q = 1$  are equal to the indices  $Max(G)$  and  $Min(G)$ , respectively.

In this paper, we compute the indices  $Max(G)$  and  $Min(G)$  and their corresponding polynomials,  $Max(G; q)$  and  $Min(G; q)$ , for some graph operations. Then, as an application of our results, we computed these indices for some familiar graphs.

**Keywords:** Wiener index, Wiener polynomial,  $Max(G)$ ,  $Min(G)$ ,  $Max(G; q)$ ,  $Min(G; q)$ , graph operations

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## ON THE NUMBER OF SMALL PATHS, INDEPENDENT SETS AND MATCHINGS OF FULLERENES

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Fullerene graphs are three–regular planar graphs with faces being pentagons and hexagons. In this talk we first compute the number of paths of low order in a fullerene. Then these numbers are used to obtain the number of independent sets and  $k$ –matchings in fullerenes for  $k = 1, 2, 3, 4$ . We have also found a relation for the Wiener polarity of a fullerene.

*Keywords:* fullerene, matching, independent set.

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## MOMENT OF INERTIA OF CHIRAL MOLECULES AS A PARAMETER FOR CALCULATING OPTICAL ROTATION: CONFORMATIONAL EFFECTS IN 2-SUBSTITUTED BUTANES

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The challenge of making a rational and general connection between the sign and magnitude of the optical rotation and molecular structure remains. In the course of our investigation on natural optical activity of organic molecules in liquid phase, we have found that the magnitude of optical rotation is correlated qualitatively and quantitatively to the moment of inertia of chiral molecules. As a continuation of our study, we wanted to see if our approach takes into consideration the conformational changes in chiral molecules (*i.e.*, as the shape of the molecule changes so does its moment of inertia and consequently the magnitude, sometimes the sign, of optical rotation). To test this we have chosen the data set from Wiberg's study on conformational effects on optical rotation in 2-substituted butanes (where X = F, Cl, C≡N, C≡CH). For each molecule conformers were generated by changing the C-C-C-C torsional angle by 20° and for the obtained geometry moment of inertia was calculated around x, y and z axes. We have managed to reproduce the Wiberg's plot<sup>1</sup> of torsional angle *vs.* calculated (*ab initio* at the B3LYP/augcc-Pvdz level) specific optical rotation. For all four molecules the shapes of the curves were similar to the ones from Wiberg's study despite the different method of calculation. We propose that the manifestation of optical activity is connected to the helical displacement of chiral molecules. The magnitude of the displacement of chiral molecule in the helical path is represented by the spherical coordinates  $r$ ,  $\theta$  and  $\varphi$ . These spherical coordinates describe the rotational and translational movement and are calculated using the moment of inertia around the three principal axes of inertia in the adopted/modified Einstein's equations to describe Brownian helical motion. Multiple regression was carried out using calculated values for  $r$ ,  $\theta$  and  $\varphi$  and correlation between Wiberg's and our calculated specific optical rotation was greater than 0.9. These results suggest that the moment of inertia of chiral molecules can be used as a parameter for calculating optical rotation.

*Keywords:* moment of inertia, optical rotation, conformational effects, 2-substituted butanes

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**ROTATIONAL MOTION AND  
THE SOLVATION PROPERTIES OF WATER –  
IMPLICATIONS FOR THE USE OF MICROWAVE IRRADIATION**

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Using Molecular Dynamics simulations in conjunction with home–developed Split Integration Symplectic Method, based on the introduction of an internal coordinate system and on the treatment of translations and rotations as vibrations with zero vibrational frequency, we are able to effectively decouple individual degrees of freedom of water molecules and to connect them to corresponding thermostats. This facilitates elucidation of structural, dynamical, spectral, and solvation properties of bulk water at any given combination of rotational, translational, and vibrational temperatures. Coupling between the simulated system and the external heat baths has to be tight in order to counter the natural phenomenon of energy dissipation. Using such simulation setup we are aiming to answer important theoretical question – how much different degrees of freedom contribute to temperature dependence of structural, dynamical, spectral, and solvation properties of bulk water. It has to be stressed that our simulations provide also practical applications in the area of microwave radiation which is emitted by mobile telephony, radars, satellites, and microwave ovens and which is subject of much speculation concerning possible adverse health effects. It was, for example, shown that microwaves enhance protein folding and aggregation in the absence of bulk heating which could finally result in the development of Alzheimer's disease. Since absorption of microwaves induces rotations of polar molecules, their continuous application leads to a creation of a non–equilibrium situation with an excess of energy built up in the form of fast rotations – i.e. a non–equilibrium situation characterized by rotations governed by a higher temperature than the other degrees of freedom. Such non–equilibrium state can be readily simulated using the above–described protocol, therefore, solvation properties of bulk water were carefully examined using three typical solutes of similar size – charged potassium ion, polar water molecule, and non–polar neon atom. Hydration by rotationally hot bulk water was shown to be conceptually similar to the application of a less polar and less protic solvent.

**HISTORY OF 161 YEARS OF DAILY TEMPERATURE PATTERNS  
AT ARMAGH (UK) WEATHER STATION FROM THE  
THERMOMETER POINT OF VIEW**

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Detailed analysis of thermometer based daily data for Armagh, using similarity based clustering and kNN algorithms suggests that the thermometer based daily temperature patterns of the 1990–2004 period could not be differentiated from the oldest temperature patterns going back to 1844. The minimum distance found in Euclidean space between two most similar years, out of 161 years in total, is 80.6 which indicate average daily variations at 3.2 °C. Two artificially created annual temperature scenarios were created to calibrate proprietary clustering algorithm and test whether either the Hockey Stick scenario or linear warming scenario could be detected in the experimental data. A systematic look at all possible pairwise comparisons between any of two years in 161 years dataset strongly suggests that neither scenario is realistic. In addition, it will be demonstrated that the use of averaging in trend analysis of warming or cooling is possibly the worst statistical tool to be used, and yet, annual averages have been used as the main indicator of global warming.



## **AutoGraphiX III: OVERVIEW OF THE NEW SYSTEM**

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About 10 years after AutoGraphiX–2 was started, a completely new version of the system is being developed. The whole code has been completely rewritten. AutoGraphiX III is based upon a different graphical interface that allows a better interaction with the software. The optimizer at the heart of the program takes advantage of the adaptive local search from the last versions of AutoGraphiX 2 but also has some major improvements at different levels. The most important one is the way to keep the search within special classes of graphs such as regular graphs or chemical graphs (graphs with maximum degree less than or equal to 4). Instead of restricting the search by the mean of constraints, these classes of graphs are directly handled by the software. It is easier to use and much more efficient as the transformations used in the local search are now selected to keep implicitly remain within the chosen class. Another improvement is from the numerical point of view as the constraints are now handled separately instead of being added to the objective function value as a penalty. Some problems that were impossible to model in AGX–2 may now be solved. During this talk, we will present the differences between the different versions of AGX and describe how to use the new system to take advantage of its new features.

## SHELL MODEL OF ASSEMBLIES OF EQUICHARGED PARTICLES SUBJECT TO RADIAL CONFINING POTENTIALS

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A shell model of an assembly of  $N$  equicharged particles subject to an arbitrary radial confining potential  $N W(r)$ , where  $W(r)$  is parameterized in terms of an auxiliary function  $\Lambda(t)$ , is presented. The validity of the model requires that  $\Lambda(t)$  is strictly increasing and concave for any  $0 \leq t \leq 1$ ,  $\Lambda'(0)$  is infinite, and  $\mathcal{A}(t) = -t^{-1}\Lambda'(t)/\Lambda''(t)$  is finite at  $t = 0$ . At the bulk limit of  $N \rightarrow \infty$ , the model is found to correctly reproduce the energy per particle pair and the mean crystal radius  $R(N)$ , which are given by simple functionals of  $\Lambda(t)$  and  $\Lambda'(t)$ , respectively. Explicit expressions for an upper bound to the cohesive energy and the large- $N$  asymptotics of  $R(N)$  are obtained for the first time. In addition, variational formulation of the cohesive energy functional leads to a closed-form asymptotic expression for the shell occupancies. All these formulae involve the constant  $\xi$  that enters the expression  $(\xi/2)n^{3/2}$  for the leading angular-correlation correction to the minimum energy of  $n$  electrons on the surface of a sphere with a unit radius (the solution of the Thomson problem). The approximate energies, which constitute rigorous upper bounds to their exact counterparts for any value of  $N$ , include the cohesive term that is not accounted for by the mean-field (fluid-like) theory and its simple extensions but completely neglect the surface-energy correction proportional to  $N$ .

## **PHOTOCHEMICAL POLLUTION LEVEL ASSESSMENT OVER THE UK BASED ON OZONE DATA 1990–2006**

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Ozone data from the UK automatic monitoring network for 13 rural and 7 urban sites for the April through September season in the years 1996–2006 have been analyzed on the basis of recently introduced photochemical pollution indicators. The indicators predict the urban sites as prone to photochemical pollution although the average ozone concentrations might be lower or the excess times above a threshold value might be higher than in some rural sites. A good correlation, however, exists with the shape of the frequency distribution of ozone concentrations, especially with the frequency of measured very low (close to zero) concentrations. Compared with similar assessment of photochemical pollution in the Central Europe and the Mediterranean (Italian, Croatian, Slovenian) region the present analysis shows that photochemical pollution problems in the UK are significantly less likely.

## **COUNTING CONJUGATED CIRCUITS IN BENZENOID CHAINS**

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We present explicit formulas for the total number of conjugated circuits of a given length in polyacene and fibonacene chains and analyze asymptotic behavior of the expected number of conjugated circuits in long chains of the considered types.

## ON THE SYMMETRY OF (3,6)–FULLERENES

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A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. A (3,6)–fullerene is a planar three regular graph with 4 triangles and  $n/2 - 2$  hexagons as faces.

In this work, symmetry properties of some (3,6)–fullerenes are determined.

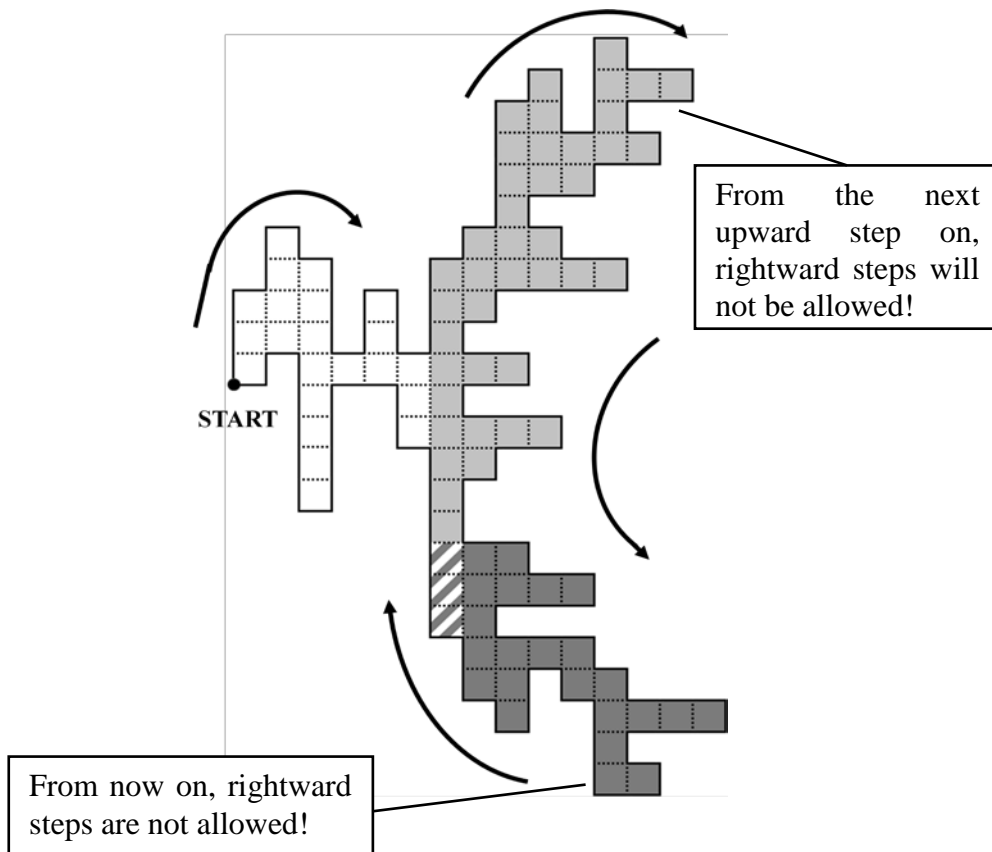
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## GENERATING FUNCTIONS FOR TRI-WALL POLYGONS

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Let  $P$  be a self-avoiding polygon with a connected leftmost column. Let  $c$  be the bottom cell of the leftmost column of  $P$ . Imagine that we start walking from the lower left corner of  $c$ , and we walk clockwise along  $P$  until we come to the starting point again. Let us write our walk as  $w_1\bar{x}w_2$ , where  $\bar{x}$  denotes the first leftward step of the walk. Now, the polygon  $P$  is a *tri-wall polygon* in two cases. One case is that  $w_2$  makes no upward steps. The other case is that  $w_2$  makes one or more upward steps, but once  $w_2$  has made its first upward step,  $w_2$  never more makes a rightward step. An example of a tri-wall polygon can be seen in the figure above.

Tri-wall polygons are a superset of column-convex polygons. The area generating function of tri-wall polygons is a rational function, and the number of  $n$ -celled tri-wall polygons behaves asymptotically as  $0.4217 \cdot 3.2056^n$ . By comparison, the number of  $n$ -celled column  $w_2$  convex polygons behaves asymptotically as  $0.1809 \cdot 3.2056^n$ . The perimeter enumeration of tri-wall polygons is still undone. I hope to do it by the conference date. I expect that the perimeter generating function is algebraic and satisfies an equation of a pretty high degree (perhaps 16).

## PHOTOPHYSICAL AND PHOTOCHEMICAL PROPERTIES OF METHOXY CURCUMINOIDS AND THEIR $\text{BF}_2$ -DERIVATIVES

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In the past decade, photochromic materials have received much attention because of their ability to function as potential photoswitchable molecular devices and optical memory storage systems.<sup>1</sup>

Piezochromism or mechanochromism refers to the colour change of materials in response to pressure or other mechanical stimuli. These colour changes are often highly dependent on the solid-state morphology and can be induced by material structural changes such as bond breaking or forming on the molecular level.<sup>2</sup>

Maximum of absorption and emission bands in UV–Visible spectra are depended on type and position of substituents. We are interested in compounds with  $\beta$ -diketone moiety<sup>3</sup> for example on curcumin, which has several very interesting bio–pharmacological activities. For that reason we prepared all isomers of dimethoxy curcuminoids in order to evaluate the effect of position of methoxy groups on the photophysical and photochemical properties.

We also determined that photostability of curcuminoids is strongly influenced by the position of methoxy group and their lifetime varied from 14.5 min in the case of 3,5–dimethoxy derivative to 287.0 min in the case of 2,5-derivative. All compounds exhibit very interesting photochromic properties and some of them also solvatochromic and mechanochromic properties.

We have also prepared  $\text{BF}_2$  derivatives of curcuminoids. Introducing  $\text{BF}_2$  as a strong electron withdrawing group changed both, photophysical and photochemical properties of curcuminoids.

In this presentation we would present some of the studied curcuminoids and their  $\text{BF}_2$  derivatives.

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## A NOTE ON VERTEX TRANSITIVE GRAPHS

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A bijection  $\sigma$  on vertex set  $V$  of graph  $G = (V, E)$  is named an automorphism of  $G$  if  $\sigma(e) = \sigma(u)\sigma(v)$  is an edge of  $E$  for every edge  $e = uv$  of the edge set  $E$  of  $G$ . Here we study automorphisms of vertex transitive graphs. Also the values of some topological indices based on eccentricity are computed. The work presented here is continuation of research presented in the *References*.

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## IDENTICAL, SIMILAR, OR DIFFERENT: QUANTIFICATION OF PSEUDOSYMMETRY RELATIONSHIPS IN MOLECULAR CRYSTALS

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In this talk we will explain how Avnir's CSM method was extended for quantification of crystallographic pseudosymmetry.  $RmS(G)$  measurements of distortion from ideal  $G$  symmetries were developed for pure translation, screw rotation, and glide reflection, as well as point group symmetries. Pseudosymmetrical independent molecules in the asymmetric unit imply that *structurally similar diastereomers mimic pairs of homomers or enantiomers* and show a particular intermolecular spatial orientation approximating symmetry. This may enable the space filling in such a crystal to emulate higher order space group packing efficiency while symmetry breaking interactions are simultaneously allowed to exist. It will be demonstrated that low  $rmS(i)$  and  $rmS(n\text{–}glide)$  values for a *kryptoracemate*  $P2_1$  chiral crystal structure (below) affords very high fidelity for the emulation of higher order  $P2_1/n$  achiral space filling.

About 90% of the time, crystallization of a racemic mixture of organic compounds yields achiral crystals known as solid–state *racemic compounds*. Only about 10% of all racemic mixtures of organic compounds crystallize as *conglomerates of chiral crystals* [simple mechanical mixtures of Sohncke space group (+)– and (–)–chiral crystals in a 1:1 statistical ratio]. Usually, only one molecule resides in the asymmetric unit ( $Z' = 1$ ) of these chiral crystals. Dissolution of one crystal excised out of the bulk results in a solution containing an enantiomerically pure compound. Two molecules in the asymmetric unit ( $Z' = 2$ ) occur when it is difficult, by symmetry alone, to simultaneously satisfy both the criteria of close packing and the requirements of optimal intermolecular interactions. Conglomerates of chiral crystals containing two symmetry unrelated molecules of opposite handedness are referred to as *kryptoracemates* or *false conglomerates*. Reports of these crystal types are relatively few: only 181 organic kryptoracemates are in the CCDB (2010). False conglomerates differ from true conglomerates in that dissolution of one chiral crystal excised out of the bulk will now produce an optically inactive solution of solvated enantiomers. When the conformations in these crystals are the same, it is often possible to observe that the independent molecules are related to one another by approximate symmetry transformations (*pseudosymmetry*).

## **SOLVABLE SUBSETS OF SELF–AVOIDING WALKS AND POLYGONS**

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Unfortunately the problem of counting self–avoiding walks (SAW) and polygons (SAP) on lattices in two dimensions or more has not been solved. However there are many proper subsets of SAW and SAP which are solvable. The study of these solvable models is based on the hope that they still retain most important features of the original model. In these talks we will review some of the solved models, include row convex, convex, prudent, spiral, quasi–prudent and perimeter walks and polygons.

We will also discuss the issue of what is an appropriate metric to decide how close a solvable model is to the original problem.

## **LATTICE GREEN FUNCTIONS AND SPANNING TREES**

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I will discuss the calculation of lattice Green functions for lattices in dimensions higher than 3, which then reveal some interesting connections with both number theory and certain differential equations that arise in string theory. Then I consider the problem of calculating the number of spanning trees on a lattice. By generalizing that calculation we make connections with lattice Green functions, and again to some problems in number theory, through the intermediate mechanism of logarithmic Mahler measures.

## **ON SOME TOPOLOGICAL INDICES AND RELATED POLYNOMIALS FOR A FAMILY OF DENDRIMERS**

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Dendrimers are large and complex molecules with very well-defined chemical structures. A topological index of graph  $G$  is a numerical quantity assigned to  $G$  and used to describe molecular graphs. The Szeged, connectivity, GA, Zagreb and PI indices are some of important topological indices applicable in nanoscience. In this paper, we focus our attention to achieve these indices for polyaryl dendrimers.

*Keywords:* nanostar dendrimer, Szeged index, connectivity index, GA index, Zagreb index, PI index

## THE HOSOYA POLYNOMIAL OF A $TUC_4C_8(S)$ NANOTORUS

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The Hosoya polynomial of a connected graph  $G$ ,  $H(G, x)$ , is defined as follows:

$$H(G, x) = \sum_{\{u,v\} \in V(G)} x_G^{d(u,v)}$$

where  $V(G)$  is the set of vertices of  $G$  and  $d(u,v)$  is the distance between a pair of vertices  $u$  and  $v$  in  $G$ . The Hosoya polynomial has many chemical applications. Two well-known topological indices, *i.e.*, Wiener index and hyper-Wiener index, can be directly obtained from this polynomial. In this paper, we compute the Hosoya polynomial of  $TUC_4C_8(S)$  nanotours by a MAPLE program.

**PROFESSOR SEAN P. McGLYNN:  
25+ YEARS WITH HIM AT LSU**

Leo KLASINC

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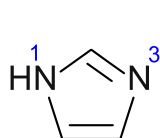
Author's reflections and memories on the time spent on sabbatical and later as a Visiting Professor at the Chemistry Department of Louisiana State University (LSU) in Baton Rouge with special emphasis on this year honoree Professor Sean McGlynn will be remembered and evocated to the participants.

## DFT STUDY OF INTERACTION OF AZOLE CORROSION INHIBITORS WITH Cu(111) SURFACE

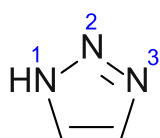
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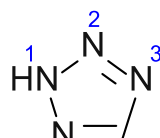
Corrosion inhibitors are substances that protect metals against corrosion by decreasing the rate of corrosion processes. Efficient inhibitors are heterocyclic organic compounds consisting of a  $\pi$ -system and/or O, N, P, or S heteroatoms. Azoles are among the popular organic inhibitors against corrosion of copper. As the adsorption of inhibitor molecules onto the surface is regarded as an important step in the formation of protective film on the surface, we studied the adsorption of plain azole molecules – imidazole, triazole, tetrazole and pentazole – on Cu(111) surface by means of atomistic computer simulations based on ~~density functional~~ <sup>density functional</sup> theory and plane-wave pseudopotential method. The aim is to determine how the number of nitrogen atoms in azole ring affects the interaction between inhibitor molecule and copper surface. Our results show that all four molecules adsorb perpendicular to the Cu(111) through nitrogen atoms. Magnitude of adsorption energy, which is of the order of 0.5 eV, decreases linearly with increasing the number of nitrogen atoms in azole ring. Trend of adsorption energy can be explained by molecular electronegativities: the smaller is the electronegativity of the molecule the larger is its charge donation to the surface: imidazole ( $0.15 e^-$ ), triazole ( $0.10 e^-$ ), tetrazole ( $0.09 e^-$ ), and pentazole ( $0.05 e^-$ ). The inspection of charge density difference reveals that in addition to N–Cu bond the molecules interact with the surface also with the bottommost H atoms (N–H  $\cdots$  Metal hydrogen bond) as seen by charge accumulation located in between them and the surface.



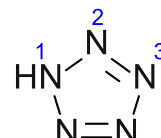
imidazole



1,2,3-triazole



tetrazole



pentazole

## SIMULATION OF LARGE MULTI-ATOM VACANCIES IN DIAMOND

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In diamond more than 500 electronic and more than 150 vibrational optical centers have been documented. Many of them are  $V_n$  vacancy centers due to missing of  $n$  neighboring carbon atoms from the diamond lattice. The number of all possible  $V_n$  vacancy clusters increases faster than exponentially as the function of the missing number  $n$  of carbon atoms. The number of these clusters goes like 1, 1, 88, 8112, 937194 for  $n = 1, 3, 7, 10, 13$ . We present an algorithm for generating all possible  $V_n$  vacancy structures up to  $n = 7$  and we calculated also their relaxed geometries and electronic structures.<sup>1,2</sup> For  $n = 8$  up to  $n = 14$  we systematically generated a large number of vacancy clusters and obtained their energies and pointed to highly stable structures among them.

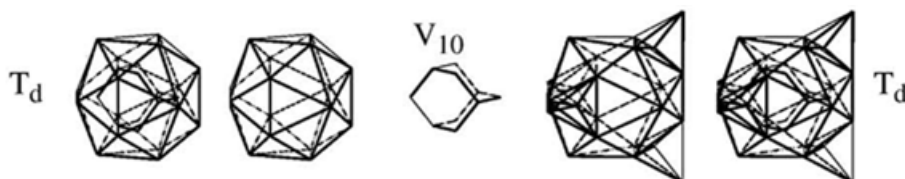


Figure 1. The geometric structure of the  $V_{10}$  vacancy cluster before and after the relaxation.

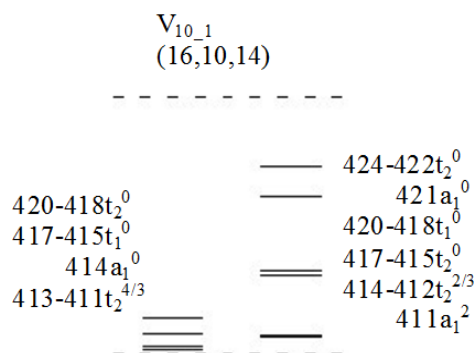


Figure 2. The electronic structure of the  $V_{10}$  vacancy cluster before and after the relaxation. Here the one-electron energy levels with their symmetry, serial numbers and occupation numbers are shown in the gap of the diamond.

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## FAMILIES OF DISTANCE–BALANCED GRAPHS

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A connected graph is distance–balanced (also called self–median) if the sum of the distances from a vertex  $v$  to all other vertices is the same regardless of the selected vertex  $v$ . Distance–balanced graphs are connected to chemistry via the Szeged index since 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.

Since the complexity of obtaining a distance–balanced graph by adding the fewest amount of edges is NP–hard, we will look at some families of graphs that are themselves distance–balanced, explore product graphs of distance–balanced graphs and present the connection to strongly distance–balanced graphs.

We will also show that bipartite distance–balanced graphs that are not even cycles or  $K_2$  have a minimal degree 3. We will conclude with some open problems on characterization of general distance–balanced graphs.

## ATOM–BOND CONNECTIVITY INDEX OF SOME NANOSTARS

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The recently introduced atom–bond connectivity (*ABC*) index has been applied up to now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined for a graph  $G$  by

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

where the summation goes over all edges of  $G$ ,  $d_u$  and  $d_v$  are the degrees of the terminal vertices  $u$  and  $v$  of edge  $uv$ . The *ABC* index has proven to be a valuable predictive index in the study of the heat of formation in alkanes.

In this article an attempt has been made to compute these indices for three types of dendrimer nanostars. Dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a stepwise fashion from simple branched monomer units. The nanostar dendrimer is a part of a new group of macromolecules that behave as photon funnels and artificial antennas.

*Keywords:* atom–bond connectivity index, dendrimer nanostars

## **$k$ –DOMINATION ON HEXAGONAL CHAIN CACTI**

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In this paper we use the concept of  $k$ –domination, where  $k$  is an integer which is greater or equal to 2. We determine minimum  $k$ –dominating sets and  $k$ –domination numbers of three special types of hexagonal cactus chains. Those are para–, meta– and ortho–chains.

For an arbitrary hexagonal chain  $Gh$  of length  $h$  we establish the lower and the upper bound for  $k$ –domination number. As a consequence, we find the extremal chains due to  $k$ –domination number.

## SEVENTY YEARS OF SCIENCE: A RETROSPECTIVE

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The foray into *Chemical Physics* began in 1952. However, prior to that time, there were a series of formative events, some comical and some depressing. These will be discussed briefly.

The story starts with triplet (T) states of molecules as initially proposed by Lewis and Kasha. In 1952, Chris Reid of Vancouver published a series of papers which called the triplet proposal into question. The resolution of the problem raised by Reid will be detailed and will involve a discussion of the triplet states of polyacenes, spin–orbit coupling, internal and external heavy–atom effects, charge transfer (CT) states, the modulation of CT and T states, triplet–triplet annihilation, excimer states, *etc.*

Discussion will then switch to the electronic structure of the Uranyl and Trans–Uranyl ions which, at that time, were hot–button issues. In particular, the phosphorescence characteristics of these ions will be emphasized. This will be followed by a review of the spectroscopy and electronic structure of a host of other ions, with some emphasis on Nitrite, Nitrate and Permanganate.

Molecular Rydberg states, ways of identifying them and algorithms for ordering them, their investigation by absorption spectroscopy and optogalvanic effects, their *giant* states, *etc.* will be discussed.

The lecture will end on a theoretical note. Given adequate time, the following topics will be investigated:

A. Is there any symmetry in the mapping that takes one from codons to amino acids? If there is, can one formulate a genetic cosmology based on it?

B. Can one formulate symmetry–adapted space–spin wavefunctions for complex molecules? If so, does any benefit accrue?

C. Can one associate genetic damage at the molecular level with the type of radiation which caused it?

D. Is there a simple way, one not invoking Hermite analysis, to deduce bond lengths from vibrational progressions?

## **BFFT APPROACH OF U(1) MASSIVE BOSON IN NON-COMMUTATIVE SPACE**

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In this article, BFFT formalism of Proca model in non-commutative (NC) space has been investigated. Considering that all theories with first class constraint are gauge theories, Proca model in non-commutative space is not a gauge theory in general due to appearance of second class constraints in it. In this work, the classical Proca model have been converted into a gauge theory using BFFT approach by introducing several auxiliary variables which in turn manage to convert the second class constraints to first class ones.

The system with constraints are described by Dirac that named Hamiltonian constraint system, two kind of first class and second class constraint play the main role in Hamiltonian constraint system. In general first class constraints theories are gauge theories but appearance of second class constraints made a difficulties . BFFT formalism convert second class to first class constrain by introducing auxiliaries variable.

Some people believe that non-commutative space appear in high energy, due to this assumption we rewrite our model in non-commutative space.

The non-commutative abelian Proca field has been rewritten as a commutative theory containing the non-commutative tensor  $\theta_{\alpha\beta}$  at the first order.

It is necessary to mentioned that Maxwell theory is a gauge theory, mass in Proca model cause to breaking of gauge invariant .

The important things that happened is when we put  $m = 0$  in non-commutative abelian Proca model. Yet we have a gauge theory and non-commutativity never lead to second class constraints and, in our theory, keeps a structure of constraints .

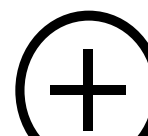
But, as we mentioned, non-commutative Proca model has second class constraint. With BFFT method we convert second class constraints to first class by introducing some auxiliary variables. After this procedure, all constraints are the first class and we have and we have a gauge theory that it is ready to quantize.

**A DFT STUDY OF THE SOLVENT EFFECTS ON THE  
MECHANISM, REGIO– AND STEREOSELECTIVITIES OF  
1,3–DIPOLAR CYCLOADDITION OF  
C–DIETHOXYPHOSPHORYL–N–METHYLNITRONE WITH  
SUBSTITUTED ALKENES**

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The molecular mechanism, *ortho/meta* regioselectivity, *endo/exo* stereoselectivity and solvent effects of 1,3-dipolar cycloaddition of C–diethoxyphosphoryl–N–methylnitron with substituted alkenes (scheme)<sup>1</sup> were analyzed using DFT method at B3LYP/6-31G(d, p) level of theory.<sup>2</sup> Analysis of the geometries of the stationary points in the gas phase<sup>3</sup> show that the reactions take place along an asynchronous concerted mechanism and favor the formation of the *ortho–endo* cycloadduct. The inclusions of solvent effects<sup>4</sup> decrease the asynchronicity of the mechanism, leading to more stereoselectivity of these 1,3–dipolar cycloaddition reactions.



*Scheme.* 1,3–dipolar cycloaddition of C–diethoxyphosphoryl–N–methylnitron with substituted alkenes.

**Keywords:** 1,3–dipolar cycloaddition, regioselectivity, stereoselectivity, mechanism, solvent effects, DFT calculations

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## ANTHOCYANINES ANTIOXIDANT ACTIVITY BY COMPUTATIONAL METHODS

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Anthocyanines are natural pigments, glycosides of anthocyanidines, compounds that have the base structure the flavilium cation moiety connected to a sugar fragment, usually at the hydroxyl in 3. Sometimes the sugar fragment may be connected to the hydroxyl in 7 position of the skeleton (Figure 1).

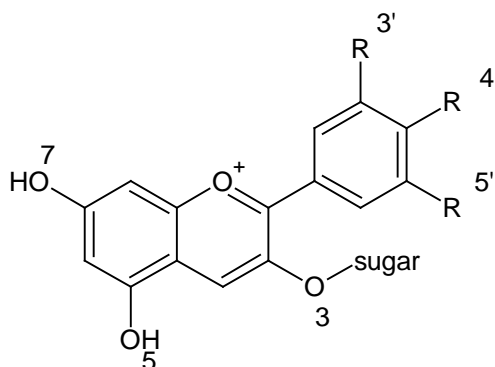


Figure 1. Anthocyanine structure

One of the main properties of this compounds is the antioxidant capacity<sup>1</sup> explained in a first approximation by the HOMO orbital energy. But this is not the single molecular descriptor that may fit the antioxidant activity.<sup>2</sup> This paper tries to present also others descriptors (hardness, electronegativity, electrophilic index and frontier density of HOMO) for five cyanidine glycosides, compare them to the same descriptors of ascorbic acid and evaluate the correlation with their antioxidant activity.

This work is part of the project 52145/2008 SAHASA carried out under the 4<sup>th</sup> Program Partnerships in Priority Areas of the National Plan for Research–Development and Innovation, 2007–2013 (Romania).

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**THE 300<sup>TH</sup> ANNIVERSARY OF THE BIRTH OF  
RUĐER JOSIP BOŠKOVIĆ  
A FAMOUS CROATIAN PHILOSOPHER AND SCIENTIST**

Krunoslav PISK

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## ELECTRONEGATIVITY AND CHEMICAL HARDNESS: RELIABLE QUANTUM TOOLS FOR CHEMICAL STRUCTURE AND REACTIVITY

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Six levels for emphasizing the electronegativity and chemical hardness as quantum chemical structure and reactivity workable tools are reviewed:

- the analysis of their quantum definitions in Fock space;
- their reliability in providing atomic patterns of periodicity within density functional softness theory;
- their atomic periodicity formulation as the semiclassical quantum propagator/Green function based theory;
- finite difference up to spectral like resolution methods based on ionization potential and electronic affinity, in providing viable relationships with other aromaticity energetic, magnetic, topologic and geometric criteria;
- their pattern sensitivity to the media or solvent effects;
- the possibility in assessing them within quantum parabolic energetic effect that closely resemble other  $\pi$ -equivalent energy expressions within the semi-empirical computation framework as better as the carbon-based system increases its complexity.

As a consequence the associate hierarchy of principles in chemical bonding is established and the idea of *chemical orthogonal space* having electronegativity and chemical hardness as main vectors is advanced.

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## RING CURRENTS IN POLYCYCLIC SODIUM CLUSTERS

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In the recent paper<sup>1</sup> the synthesis and structure of a *fac*-trioxo molybdenum metalloligand and its sodium complex containing 1D hexagonal chains of sodium ions has been reported. In the same work, the aromaticity of hexagonal Na clusters has been quantified by means of the nucleus-independent chemical shift and electronic multicentre indices. It has been shown that the aromaticity of hexagonal Na-clusters is of the same order as the aromaticity of analogous benzenoid hydrocarbons.

In the present study the aromaticity of polycyclic Na-clusters was analyzed using current density maps computed by means of coupled HF theory using the diamagnetic-zero variant of the continuous transformation of origin of current density (CTOCD-DZ) method. It was shown that although polycyclic Na-systems sustain a diatropic ring current, the induced current density is several times weaker than in analogous benzenoid hydrocarbons. A detailed analysis revealed that the current density in hexagonal Na-systems is almost completely determined by four HOMO  $\sigma$ -electrons.

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## **A FAST APPROACH TO THE DETECTION OF ALL–PURPOSE HUBS AND COMMUNITIES IN COMPLEX NETWORKS**

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A novel algorithm for the fast detection of hubs in chemical networks is presented. The algorithm identifies a set of nodes in the network as most significant, aimed to be the most effective points for fast, widespread distribution throughout the system. We show that our hubs in general have greater closeness centrality and betweenness centrality than vertices with maximal degree, while having comparable or higher degree than vertices with greatest closeness centrality and betweenness centrality. Several theoretical and real–world chemical and biological networks are analyzed.

Additionally, the fast detection of communities in these large network systems is discussed.

**A MODEL TO ESTIMATE STABILITY CONSTANTS OF  
AMINO–ACID CHELATES WITH Cu(II) AT  
DIFFERENT IONIC STRENGTHS**

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The equation for the simultaneous prediction of stability constants at various ionic strengths for copper(II) *mono*-complexes with  $\alpha$ -amino acids was developed. It is based on valence connectivity index of the 3<sup>rd</sup> order ( ${}^3\chi^v$ ) and specific ion interaction theory (SIT). The equation was tested on the set consisted of 31  $\log K_1$  values for the complexes with four  $\alpha$ -amino acids (glycine, alanine, valine and leucine) measured at  $I = 0 - 2 \text{ mol/dm}^3$ . The theoretical values were in fair agreement with the experimental ones, with the standard error of estimate 0.09. Moreover, only two  $\log K_1$  values were reproduced with an absolute error  $> 0.2$ .

## **SYNTHESIS OF COBALT SULFIDE NANOPARTICLES BY SIMPLE HYDROTHERMAL METHOD**

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&

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Among the nanometer–scale materials metal sulfides nanomaterials have been the focus of considerable interest due to their unique optical and electrical properties and their wide variety of potential applications in nanoscale devices such as electroluminescence and nonlinear optical devices. One of these metal sulfides is cobalt sulfide. Cobalt usually forms a variety of binary sulfides with the general formula of  $\text{CoS}_x$  which have attracted great attention in virtue of their excellent properties and potential application for hydrodesulfurization and hydrodearomatization in many industrial fields.

In 2001, the hydrothermal method has been also reported to prepare metal sulfides nanostructural materials, which have potential advantages of relatively low cost, high purity, and controlled morphology. Also a mild hydrothermal route has been developed to synthesize metal sulfides with use of thioglycolic acids as nontoxic template and sulfide precursor. In present paper we report on synthesis of cobalt sulfide *via* hydrothermal method with the use of cobalt salt as a precursor for Co and thioglycolic acids for S. To the best of my knowledge this is the first report of synthesis of cobalt sulfide nanocrystals by the simple precursors via hydrothermal method. In a typical synthesis different molar ratios of  $\text{Co}(\text{AC})_2$  and thioglycolic acid were mixed in 200 mL distilled water under stirring. The final mixed solution was heated at different temperature for 24–48 h and then was cooled to room temperature. The best condition was selected by computation. The products were characterized by X–ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared (FT–IR) spectra. Optical property of obtained products was investigated by photoluminescence (PL) spectroscopy.

## ON ORDERING ALKANES BY MODIFIED ZAGREB INDICES

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The topological Zagreb index  $M_1$  introduces an ordering on the set of alkanes. Recently, modified Zagreb indices  ${}^\lambda M_1$  have been proposed, and it is noted that they differently order alkanes. In this paper, the level of consistency between these orders is analyzed. A new partial order  $\succ$  as the intersection of all partial orders  ${}^\lambda M_1$  (where  $\lambda$  is at least 2) is introduced and its properties are analyzed.

## COMPUTING CONSTANTS IN SOME SUBSPACES OF FREE UNITAL ASSOCIATIVE COMPLEX ALGEBRA

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We consider a free unital associative complex algebra  $B$  generated by  $N$  generators, each of degree one. We equip  $B$  with a multiparametric  $q_{ij}$ -differential structure given by  $N$  linear operators, which generalise partial derivatives. The algebra  $B$  is graded by total degree. More generally  $B$  could be considered as multigraded. Then it has a direct sum decomposition into multigraded (weight) subspaces  $B_Q$ , where  $Q$  runs over multisets (over  $N$ ). When  $Q$  is a set, the associated weight subspace  $B_Q$  is called generic, otherwise  $B_Q$  is called degenerate. An element  $C$  in  $B$  is called a *constant* if it is annihilated by all generalized partial derivatives. Then the main problem is to describe the space of all constants in  $B$ . By using the decomposition of  $B$  into multigraded weighted subspaces  $B_Q$  the main problem reduces to finding constants in each  $B_Q$ . Up to total degree equal to four we give explicit formulas for basic constants in  $B_Q$ . Depending on the actual (singular) values of parameters  $q_{ij}$ 's the number of basic constants in  $B_Q$  may vary as well.

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## HYPERBOLIC ANALOG OF THE EASTWOOD–NORBURY FORMULA FOR ATIYAH DETERMINANT

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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 (Atiyah, Eastwood & Norbury, Đoković). In a lengthy preprint (Svrtan & Urbiha, 2006) 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 (2001) found an intrinsic formula for the Euclidean 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 the Euclidean three space.

So far we also get a polynomial formula (for five points) and have an existence proof of a polynomial formula for all planar configurations what was conjectured by Eastwood and Norbury (2001). The aim of this talk is to present, for the first time, a hyperbolic analog of the Eastwood–Norbury formula for arbitrary four points in a hyperbolic plane.

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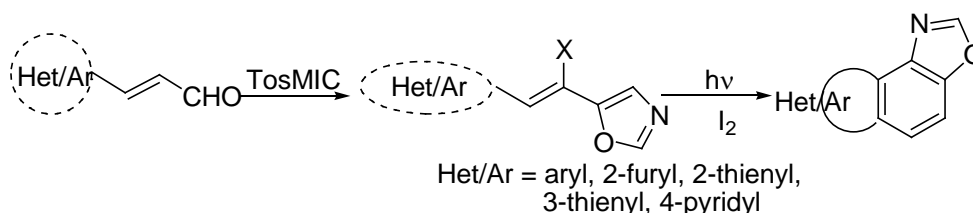
**PHOTOCHEMICAL APPROACH TO NAPHTHOXAZOLES AND  
FUSED HETEROBENZOXAZOLES FROM  
5-(PHENYL/HETEROARYLETHENYL)OXAZOLES**

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A new synthetic approach is presented for the synthesis of naphthoxazoles and fused heterobenzoxazoles. The starting 5-(aryl/furyl/thienyl/pyridyl ethenyl)oxazoles are prepared from the corresponding  $\alpha,\beta$ -unsaturated aldehydes using Van Leusen reagent in very good yields and are transformed into naphthoxazoles and fused heterobenzoxazoles on irradiation under aerobic conditions and in the presence of iodine.



All new compounds are characterized by spectroscopic methods. As the starting aldehydes for the reactions with TosMIC were all in trans configuration the obtained 5-aryl/heteroaryl-ethenyl-oxazoles retained the trans configuration which is clearly seen from the coupling constants of ethylene protons ( $J = 16$  Hz) in <sup>1</sup>H NMR. It is interesting that H-2 and H-4 oxazole protons of all Ar/Het-ethenyl-oxazole derivatives appear at the same  $\delta$  values, around 7.8 and 7.1 ppm, respectively. The two ethylene protons were also found in all examples in a similar narrow region as two doublets at 6.7–7.0 and 6.9–7.1 ppm, respectively.

**APPROACH FOR VALIDATION OF GEOLAND2 PRODUCTS  
USING PASTiS 57 (AUTONOMOUS LIGHT SENSORS FOR  
PAI CONTINUOUS MONITORING):  
BIOPHYSICAL PRODUCTS TRENDS OVER EUROPE**

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Geoland–2 BioPar version 1 product, called GEOV1, includes validation of several vegetation parameters which include leaf area index (LAI), the fraction of absorbed photosynthetically active radiation (FAPAR), and the fraction of vegetation cover (FCOVER), as well as the NDVI vegetation index. The main goal is to create high spatial resolution maps of biophysical variables using remote sensing (satellite imagery) data and then validate the maps using field measurements. Mapping of the medium and fine resolution sensors have become a unique source of information to characterize land surface properties providing the inputs required by ecosystem and climate models. For field measurements we use autonomous light sensors for plant area index (PAI) continuous monitoring (PASTiS 57). The system is aiming at continuously recording canopy transmittance in a particular configuration that should minimize the effect of: leaf area distribution, leaf clumping and illumination condition, which commonly cause variations in reflectance and thus, may cause high variability in the final products/maps of vegetation parameters.

The system is composed of a data logger where six sensors are connected with wires. The sensors are based on LEDs sensitive to the blue spectral domain. Using the blue domain allows to minimize the effect of the illuminations conditions, particularly when the sensor is not looking directly toward the sun. The sky is relatively bright in the blue domain, because of the Rayleigh and aerosol scattering. Contrary, vegetation elements show very low values of reflectance and transmittance in this spectral domain where absorption by pigments and several molecules is very high (Baret *et al.*, 2010). The contrast between the sky and the vegetation elements will be therefore maximal in this domain.

The sensors are oriented at 57.5° towards the north. This geometrical configuration allows minimizing the effect of the illumination conditions, as well as the effect of leaf angle distribution and clumping. The sensors are equipped with a nail allowing fixing it directly in the soil.

The satellite data includes fine spatial resolution data such as SPOT HRV and FORMOSAT 2. The vegetation parameters products/maps will be created using various algorithms and the validation of the maps will be performed using PASTiS 57. Four main study sites include crop fields in Barrax (Spain), La Crau (France) and Poznan (Poland), and a forest site HyyTiala located in South France. Quantitative uncertainties of GEOV1 and reference products will be computed against reference data representative of an area of 3x3 km and accounting for upscaling effect of satellite imagery. Difference maps with regional product and root mean square error maps (RMSE) will be analyzed over the period.

## COMPUTING THE ENERGY OF TWO TYPES OF DENDRIMERS

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Dendrimers are large and complex molecules with very well-defined chemical structures. They consist of three major architectural components: core, branches and end groups. Nanostar dendrimers are part of a new group of macromolecules. The energy of a graph is the sum of absolute values of all graph eigenvalues. Computing the energy of two types of dendrimers is the aim of this article.

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## **SELF-AVOIDING WALKS**

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Self-avoiding walks are walks on a (regular) lattice which do not intersect themselves. They appear in graphical expansions of quantities in the Ising model and as models of linear polymers in solution in good solvents. A natural first question is to ask for the number of self-avoiding walks (starting at the origin, or counted modulo translation) on a particular lattice with a certain number of steps.

These lectures will review what is known rigorously about these objects and will discuss several open questions. In a certain sense we know the answers but rigorous results are very hard to obtain. We shall also discuss some extensions of the questions about self-avoiding walks to other objects such as lattice polygons (embeddings of the circle graph in a lattice). For the polygon case there are interesting questions involving topological constraints. For instance, in three dimensions the polygon can be knotted. What can we say about knot probabilities or about relative frequency of occurrence of different knot types? The emphasis will be on what is known rigorously and on some open questions. By adding interactions to the walk (or polygon) it is possible to adapt the model to describe phenomena such as polymer adsorption and this area will also be reviewed.

Ideas from analysis, combinatorics and algebraic topology will appear in the lectures but very little background will be assumed.

## **COMBINATORIAL MODELS IN POLYMER PHYSICS**

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Directed walks such as Dyck and Motzkin paths are useful, exactly solvable, models of polymer adsorption and they can be adapted to model the way in which the polymer desorbs under the influence of a force. Under certain solvent conditions polymers can collapse to a compact ball. This transition can be modelled by partially directed walks and the model can be adapted for the case where a force is applied. Recent progress will be discussed.

## ENHANCEMENT OF THERMAL TRANSPORT IN CORRELATED MULTILAYERS

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We present the results for the charge and heat transport in inhomogeneous multilayers with correlated electrons. The device consists of several weakly correlated metal planes sandwiched between two semi-infinite Mott insulators.

The electron dynamics of the device is described by the Falicov–Kimball model which is solved by an inhomogeneous DMFT algorithm.<sup>1</sup> By varying the number of planes in the mid-section we can change the effective dimensionality of metallic electrons. By increasing the correlation strength we can bring the mid-section in the proximity of the MI transition and enhance the slope of the density of states close to the chemical potential. Both effects are supposed to have a large impact on the thermoelectric properties of the device.

For the macroscopic currents flowing parallel to the multilayer planes, we calculate the transport properties by linear response theory and, thus, obtain the conductivity, the Seebeck coefficient, the power factor, and the figure-of-merit of the device.

The impact of the on-site correlations and the reduction of the dimensionality on thermal transport are considered in detail.<sup>2</sup> The effects of the gate voltage applied perpendicular to the planes are discussed as well.

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