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Extended Abstract Booklet

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Augmented Eccentric Connectivity Index

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Abstract. 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

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and The R. Bošković Institute, POB 180, HR-10002 Zagreb, Croatia

Abstract. 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 bi-lobal 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 coordinates. However, two problems appeared with this algorithm: the ends of the nanotubes turned back and the nanotubes become narrower as one moves to their tips. All the deficiencies have been finally 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. The related shape analysis was done in collaboration with Professors István László of Budapest, Hungary, and Tomaž Pisanski of Ljubljana, Slovenia.

Some possible applications of novel carbon nanostructures in biology, medicine and related fields will be also discussed.
Mathematical Meaning and Importance of the Topological Index Z

Haruo Hosoya

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Abstract. In 1971 I proposed the topological index Z for characterizing the topological structure of the carbon atom skeleton of saturated hydrocarbon molecule [1]. Later a number of researchers in mathematical chemistry proposed their own topological indices. Since the term topological index is currently used as a general name for those molecular descriptors, here let us call my own index “the Z-index.” The Z-index was found not only to correlate well with the boiling point and other thermodynamic quantities, but also to be suitable for classification and coding of hydrocarbons. Later it was also found to have good correlation with the $\pi$-electronic properties of unsaturated hydrocarbon molecules, and mathematical meaning of aromaticity in benzene-like compounds was clarified by the graph-theoretical molecular orbital theory by using the Z-index [2].

The Z-index is defined as the sum of “non-adjacent number $p(G,k)$”, which is the number of ways for choosing $k$ non-adjacent edges from a given graph G.

$$Z_G = \sum_{k=0}^{\lfloor N/2 \rfloor} p(G,k)$$  \hspace{1cm} (1)

For tree graphs it can be proved that the characteristic polynomial $P_G(x)=(-1)^N\det(A - xE)$, which is expressed in terms of the adjacency matrix $A$ and the unit matrix $E$ of the order of $N$, the number of vertices of $G$, can be expressed in terms of $p(G,k)$ as,

$$P_G(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(G,k)x^{N-2k}. \hspace{1cm} (2)$$
This property already reveals that the Z-index might be closely related to various mathematical concepts and objects. The simplest example is the graph-theoretical interpretation of the Pascal’s triangle. Namely, by rotating it by 45 degree the table of the $p(G,k)$ values of the series of path graphs, $S_N$, composed of $N$ vertices connected consecutively by $N-1$ edges, appears. The sum of $p(G,k)$’s in each row is nothing else but a Fibonacci number. Similarly, the Lucas numbers appear in the table of $p(G,k)$’s for the series of monocyclic graphs.

A caterpillar graph $C_n(x_1, x_2, \ldots, x_n)$ has been defined in the graph theory in such a way that a set of star graphs of different sizes are embedded on all the vertices of a path graph, $S_n$.

In this notation, a path graph, $S_n$, is denoted by $C_n(1, 1, \ldots, 1)$, while $C_n(2, 2, \ldots, 2)$ denotes a comb graph. The Z-indices of the set of comb graphs are Pell numbers, $1, 2, 5, 12, 29, \ldots$, with the recursion relation of

$$f_n = 2f_{n-1} + f_{n-2}.$$ \hspace{1cm} (3)

As will be shown later a number of mathematical problems were found to be interpreted by the Z-indices of caterpillar graphs [3]. For example, all the solutions of the Pell equation,

$$x^2 - D y^2 = 1,$$ \hspace{1cm} (4)

a quadratic version of the Diophantine equation, can be represented by the Z-indices of certain caterpillar graphs [4].

The following diagram shows the important role of the Z-index for connecting various algebraic and geometric properties by the aid of caterpillar graphs [5]. More detailed description for these respective problems will be given in this talk.
References


Bond Additive Modeling

Damir Vukicevic

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Abstract. 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.
Reverse Wiener Index

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Abstract. The reverse Wiener index of a connected graph $G$ is defined as

$$\Lambda(G) = n(n-1)d/2 - W(G),$$

$(n - 1)d - (G)$ where $n$ is the number of vertices, $d$ is the diameter, and $W(G)$ is the Wiener index of $G$. We survey various mathematical properties of the reverse Wiener index, including lower and upper bounds for the reverse Wiener index, characterizations of trees, unicyclic graphs, and bicyclic graphs with large and/or small reverse Wiener indices.
Oral Presentation
On the Eccentric Connectivity Polynomial of Certain Graphs

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Abstract. The eccentric connectivity polynomial of a molecular graph \(G\) is defined as
\[ ECP(G, x) = \sum_{v \in V(G)} deg(v) x^{ecc(v)}, \]
where \(ecc(v)\) is defined as the length of a maximal path connecting \(v\) to another vertex of \(G\). The eccentric connectivity index is the first derivative of \(ECP(G, x)\) evaluated at \(x = 1\). In this paper we study the eccentricity connectivity polynomial and index for certain graphs and obtain the eccentricity connectivity polynomial of an infinite family of dendrimers.

Keywords: Eccentricity connectivity polynomial, eccentricity index, dendrimer, graph

1 Introduction

A simple graph \(G = (V, E)\) is a finite nonempty set \(V(G)\) of objects called vertices together with a (possibly empty) set \(E(G)\) of unordered pairs of distinct vertices of \(G\) called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

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If \( x, y \in V(G) \) then the distance \( d(x, y) \) between \( x \) and \( y \) is defined as the length of a minimum path connecting \( x \) and \( y \). The eccentric connectivity index of the molecular graph \( G \), \( \xi^e(G) \), was proposed by Sharma, Goswami and Madan [4]. It is defined as

\[
\xi^e(G) = \sum_{u \in V(G)} \deg_G(u) \text{ecc}(u),
\]

where \( \deg_G(x) \) denotes the degree of the vertex \( x \) in \( G \) and \( \text{ecc}(u) = \text{Max}(d(x, u) \mid x \in V(G)) \), see [2,3] for details. The radius and diameter of \( G \) are defined as the minimum and maximum eccentricity among vertices of \( G \), respectively. The eccentric connectivity polynomial of a graph \( G \), \( ECP(G, x) = \sum_{v \in V(G)} \deg(v)x^{\text{ecc}(v)} \), (see [1]). Then the eccentric connectivity index is the first derivative of \( ECP(G, x) \) evaluated at \( x = 1 \).

The nano-star dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Recently some people investigated the mathematical properties of this nano-structures.

We denote the complete graph of order \( n \), the complete bipartite graph with part sizes \( m, n \), the cycle of order \( n \), the star of order \( n \), and the path of order \( n \), by \( K_n \), \( K_{m,n} \), \( C_n \), \( K_{\frac{1}{2},n} \), and \( P_n \), respectively.

In Section 2 we compute the eccentricity connectivity polynomial for some specific graphs. As a consequece we study the eccentric connectivity index for paths, cycles, trees and some another graphs. In Section 3, we compute the eccentric connectivity polynomial of an an infinite family of dendrimers.

2 Eccentricity connectivity polynomial of certain graphs

In this section we consider some specific graphs and compute their eccentric connectivity polynomials.
Theorem 1.

(i). Let \( n \geq 3 \). The eccentricity connectivity polynomial of \( C_n \) is

\[
ECP(C_n, x) = 2nx^{\left\lfloor \frac{n}{2} \right\rfloor}.
\]

(ii). Let \( n \in \mathbb{N} \). The eccentricity connectivity polynomial of \( P_{2n} \) is

\[
ECP(P_{2n}, x) = 2x^{2n-1} + 4x^{2n-2} + 4x^{2n-3} + \ldots + 4x^{n+1} + 8x^n.
\]

(iii). Let \( n \in \mathbb{N} \). The eccentricity connectivity polynomial of \( P_{2n+1} \) is

\[
ECP(P_{2n+1}, x) = 2x^{2n} + 4x^{2n-1} + 4x^{2n-2} + \ldots + 4x^n.
\]

(iv). The eccentricity connectivity polynomial of \( K_n \) is

\[
ECP(K_n, x) = n(n-1)x.
\]

(v). If \( m, n \geq 2 \), then the eccentricity connectivity polynomial of \( K_{m,n} \) is

\[
ECP(K_{m,n}, x) = 2mnx^2.
\]

Since the eccentric connectivity index is the first derivative of \( ECP(G, x) \) evaluated at \( x = 1 \), we have the following theorem:

Theorem 2.

(i) The eccentric connectivity of \( K_n, \ (n \geq \gamma) \) is \( \xi^c(K_n) = n(n-1) \).

(ii) The eccentric connectivity of \( K_{m,n}, \ (m,n \geq \gamma) \) is \( \xi^c(K_{m,n}) = \gamma mn \), and the index reaches its maximum for \( K_{m,n} \) when \( m = n = \frac{m+n}{\gamma} \).
(iii) The eccentric connectivity of the star of order \( n \geq 3 \) is \( \xi^{c}(K_{1,n-1}) = r(n-1) \).

(iv) The eccentric connectivity of the cycle is \( \xi^{c}(C_{n}) = \begin{cases} n^r & \text{if } n \text{ is even} \\ n(n-1) & \text{if } n \text{ is odd} \end{cases} \).

(v) The eccentric connectivity of the path is
\[
\xi^{c}(P_{n}) = \begin{cases} 
\frac{1}{r}(n^r - r n + r) & \text{if } n \text{ is even} \\
\frac{1}{r}(n-1)^r & \text{if } n \text{ is odd} 
\end{cases}
\]

3 Eccentric connectivity polynomial of an infinite family of dendrimers

In this section we shall study the eccentric connectivity polynomial of an infinite family of dendrimers.

Figure 1: The first kind of dendrimer of generation 1-3 has grown 3 stages
We compute the eccentricity connectivity polynomial of the first kind of dendrimer of generation 1-3 has grown $n$ stages. We denote this graph by $D_3[n]$. Figure 1 show the first kind of dendrimer of generation 1-3 has grown 3 stages ($D_3[3]$).

References


Revised Szeged Index of Graph Operations

J Asadpour\textsuperscript{1}, M. Alaeiyan\textsuperscript{2} and A. R. Ashrafi\textsuperscript{3,2}

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Abstract. Let $G$ be a graph and $x, y \in V(G)$. The distance $d(x, y)$ is defined as the length of a minimal path in $G$ connecting $x$ and $y$. A graph invariant related to the distance function $d(\cdot, \cdot)$ is called a distance-based graph invariant. Topological indices are graph invariants applicable in chemistry. Suppose $n(u; v)$ and $o(u; v)$ denote the number of vertices that are closer to $u$ than to $v$ and the number of vertices of the same distance from $u$ and from $v$, respectively. The Szeged and revised Szeged index of $G$ are defined as follows:

$$Sz(G) = \sum_{uv \in E(G)} n(u; v)n(v; u), \quad Sz^*(G) = \sum_{uv \in E(G)} \left[n(u; v) + \frac{1}{2} o(u; v)\right]\left[n(v; u) + \frac{1}{2} o(v; u)\right].$$

The aim of this paper is to study the revised Szeged index under some graph operations.

Keywords: Szeged index, revised Szeged index, graph operations.
Topological Indices of Dendrimers

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Abstract. Dendrimers are one of the main objects of nanobiotechnology. They possess a well defined molecular topology. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. A topological index is a map $\Psi$ from the class of all graphs, $\text{Graph}$, into real numbers such that $G \cong H$ implies that $\Psi(G) \cong \Psi(H)$. A distance-based topological index for a graph $G$ is a topological index related to the distance function $d(-,-): V(G) \times V(G) \rightarrow \mathbb{R}$ in which $d(x,y)$ is defined as the length of a minimal path connecting $x$ and $y$. In this talk, we report our recent results on computing distance-based topological indices of dendrimers.

Keywords: Dendrimer, distance, topological index.

References


Some Topological Indices Of Non-Commuting Graph Of Dihedral Groups

Azad$^1$ and G. H. Fath-Tabar$^2$

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Abstract. Let $G$ be a non-abelian group and let $Z(G)$ be the center of $G$. We associate with $G$ a graph $\Gamma_G$ as follows: Take $G\setminus Z(G)$ as vertices of $\Gamma_G$ and join two distinct vertices $x$ and $y$ whenever $xy \neq yx$. The graph $\Gamma_G$ is called non-commuting graph of $G$. In this paper we compute some topological indices of non-commuting graph of dihedral groups.

Keywords: Non-commuting graph, dihedral group, topological index.

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Computing Eccentric Connectivity Index Of Dendrimers

A. Azad and M. Ghasemi

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Abstract. The eccentric connectivity index of the molecular graph $G$, $\xi(G)$, was proposed by Sharma, Goswami and Madan. It is defined as $\xi(G) = \sum_{u \in V(G)} \text{deg}(u) \text{ecc}(u)$, where $\text{deg}(x)$ denotes the degree of the vertex $x$ in $G$ and $\text{ecc}(u) = \text{Max}\{d(x, u) \mid x \in V(G)\}$. In this paper this topological index is computed for some classes of dendrimers.

Keywords: Eccentric connectivity index, Dendrimers, Topological index.

Figure 1. The graph of a dendrimer.
1. Introduction

At first we recall some algebraic definitions that will be used in the paper. Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph G are denoted by V(G) and E(G), respectively. If x, y ∈ V(G) then the distance d(x, y) between x and y is defined as the length of a minimum path connecting x and y. The eccentric connectivity index of the molecular graph G, ξ(G), was proposed by Sharma, Goswami and Madan\(^1\). It is defined as
\[ ξ(G) = \sum_{u \in V(G)} \deg_G(u) \cdot \text{ecc}(u), \]
where \( \deg_G(x) \) denotes the degree of the vertex x in G and \( \text{ecc}(u) = \max\{d(x,u) \mid x \in V(G)\} \), see [2-6] for details. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. We now define the eccentric connectivity polynomial of a graph G, \( ζ(x) \), as
\[ ζ(x) = \sum_{a \in V(G)} \deg_G(a) x^{\text{ecc}(a)}. \]
Then the eccentric connectivity index is the first derivative of \( ζ(x) \) evaluated at \( x = 1 \).

References


Energy Of Graphs, Matroids and Generalized Fibonacci Numbers

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Abstract. The energy $E(G)$ of a graph $G$ is the sum of the absolute values of the eigenvalues of $G$. In this article we consider the problem whether generalized Fibonacci constants $\varphi_n$ ($n \geq 2$) can be the energy of graphs. We show that $\varphi_n$ can not be the energy of graphs. Also we prove that all natural powers of $\varphi_{2n}$ cannot be the energy of a matroid.

Keywords: Graph energy, Fibonacci numbers, Matroid

MSC: 05C50, 11B39

1 Introduction

Let $G=(V,E)$ be a simple and finite graph of order $n$ where $V$ and $E$ be vertex and edge sets of $G$, respectively. If $A$ is the adjacency matrix of $G$, then the eigenvalues of $A$, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are said to be the eigenvalues of the graph $G$. These are the roots of the characteristic polynomial $\varphi(G,\lambda) = \prod_{i=1}^n (\lambda - \lambda_i)$. An interval $I$ is called a zero-free interval for a characteristic polynomial $\varphi(G,\lambda)$ if $\varphi(G,\lambda)$ has no root in $I$. 
The energy of the graph $G$ is defined as $E = E(G) = \sum_{i=1}^{n} |\lambda_i|$. This definition was put forward by I. Gutman [4] and was motivated by earlier results in theoretical chemistry [5]. It is easy to see that if an undirected graph $G$ has only real eigenvalues and $\lambda_1, \lambda_2, \ldots, \lambda_m$ be the positive eigenvalues, then $E = \sum_{i=1}^{m} \lambda_i$.

A matroid $M$ consists of a non-empty finite set $E$ and a non-empty collection $I$ of subsets of $E$, called independent sets, satisfying the following properties:

1. any subset of an independent set is independent,

2. if $I$ and $J$ are independent sets with $|J| > |I|$ then there is an element $e$, contained in $J$ but not in $I$ such that $I \cup \{e\}$ is independent.

Let $M = (E, I)$ be a matroid defined in terms of its independent sets. Then a subset of $E$ is dependent if it is not independent and a minimal dependent set is called a cycle. If $M(G)$ is the cycle matroid of a graph $G$ then the cycles of $M(G)$ are precisely the cycles of $G$. A graphic matroid is a matroid $M(G)$ on the set of edges of a graph $G$ by taking the cycles of $G$ as the cycles of the matroid. For a subset $A$ of $E$, the rank of $A$ denoted by $r(A)$, is the size of the largest independent set contained in $A$. Note that the rank of $M$ is equal to $r(E)$ since a subset $A$ of $E$ is independent if and only if $r(A) = |A|$. Recall that a complex number $\zeta$ is called an algebraic number (respectively, algebraic integer) if it is a zero of some monic polynomial with rational (respectively, integer) coefficients (see [9]). Corresponding to any algebraic number $\zeta$, there is a unique monic polynomial $P$ with rational coefficients, called the minimal polynomial of $\zeta$ (over the rationals), with the property that $P$ divides every polynomial with rational coefficients having $\zeta$ as a zero. (The minimal polynomial of $\zeta$ has integer coefficients if and only if $\zeta$ is an algebraic integer.) Since the characteristic polynomial is a monic polynomial in $\lambda$ with integer coefficients, its zeros are, by definition, algebraic integers. This naturally raises the question: Which algebraic integers can occur as energy of a graph?
In 2004 Bapat and Pati [1] obtained the following result:

**Theorem 1.** The energy of a graph cannot be an odd integer.

In 2008 Pirzada and Gutman communicated an interesting result:

**Theorem 2.** (\([7]\)) The energy of a graph cannot be the square root of an odd integer.

Also [3] and [8] contribute to the question of which numbers can be graph energies. In this paper we prove some further results of this kind.

## 2 Energy of graph and the golden ratio

In this section, we investigate the golden ratio as a graph energy. We show that \( \tau \) cannot be a graph energy. Also we prove that all \( n \)-anacci constants cannot be a graph energy. We need the following theorem:

**Theorem 3.** ([2]) If graph \( G \) with order \( n \) has no isolated vertices, then

\[
E(G) \geq 2\sqrt{n - 1},
\]

with equality for stars.

The following theorem is an immediate consequence of Theorem 3.

**Theorem 4.** The golden ratio \( \tau = \frac{1 + \sqrt{5}}{2} \) cannot be the energy of a graph.

**Definition 1.** An \( n \)-step \((n \geq 2)\) Fibonacci sequence \( F_k^{(n)} \), \( k = 1, 2, 3, \ldots \) is defined by letting

\[
F_1^{(n)} = F_2^{(n)} = \ldots = F_{n-1}^{(n)} = 1 \quad \text{and other terms according to the linear recurrence equation}
\]

\[
F_k^{(n)} = \sum_{i=1}^{k-1} F_{k-i}^{(n)}, \quad (k > 2).
\]

The limit \( \phi_n = \lim_{k \to \infty} \frac{F_k^{(n)}}{F_{k-1}^{(n)}} \) is called the \( n \)-anacci constant.
It is easy to see that \( \varphi_n \) is the real positive zero of \( f_n(x) = x^n - x^{n-1} - \ldots - x - 1 \), and this polynomial is the minimal polynomial of \( \varphi_n \) over \( \mathbb{Z}[x] \). It is obvious that \( \varphi_n \) is a zero of
\[ g_n(x) = x^n (2 - x) - 1 \]
Note that \( \varphi_2 = \tau \), where \( \tau = \frac{1 + \sqrt{5}}{2} \) is the golden ratio, and \( \lim_{n \to \infty} \varphi_n = 2 \) (see [6]).

**Theorem 5.** For every integer \( n \geq 2 \), the \( n \)-anacci numbers \( \varphi_n \) can not be the energy of a graph.

3 2n-anacci and energy of matroid

In this section we study 2n-anacci constant as graph energy.

**Theorem 6** If \( \alpha \) is not a root of any characteristic polynomial of graph, then \( \alpha \) cannot be energy of graph.

**Theorem 7** All natural powers of \( \varphi^{2n} \) cannot be energy of matroids.

**References**


Kekuleh Structures In Nano Tubes

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Abstract: A matching M in G is a set of pairwise non-adjacent edges; that is, no two edges share a common vertex. A perfect matching in G is a matching covers all vertices of G. Therefore perfect matching is n/2 matching.

Ever since introduced by the Czech chemist Friedrich August Kekulé von Stradonitz in 1865, Kekulé valence structures have played a major role in organic chemistry. Kekule structure is the perfect matching in molecular graphs. Kekulé structures in benzenoid hydrocarbons are discussed in the famous book of Cyvin and Gutman [1]. In physics, the enumeration of Kekulé structures is equivalent to the dimer problem of rectangle lattice graph in the plane Counting Kekulé structures is a very difficult problem in chemical graph theory. Some recent techniques allowed to estimate the lower bound of this number in certain classes of graphs.

A TUC₄C₈ net is a trivalent decoration made by alternating rhombi C₄ and octagons C₈. It can cover either a cylinder or a torus. In this paper we focus our attention on the
number of Kekulé structures in TUC₄C₆(R) nanotube and a close formula is established. Also we find recursive formula for the number of Kekulé structures in some classes of nanotubes.

**Keywords**: Nanotube, Kekulé Structure, Matching.

**References**


Extremal Problem With Respect To Z Index and $\sigma$ Index for Some Prescribed Classes of Graphs

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Abstract. $\sigma$ index are typical examples of graph invariants used in mathematical chemistry. They can be used for quantifying relevant details of molecular structure. The problems of characterization of the graphs within certain prescribed classes that maximize or minimize the index value are considered by many authors. In this talk we introduce some new results about Fibonacci numbers by which we can construct some monotonic transformations for the indices. Then we solve the extremal problems with respect to Z index and $\sigma$ index for some prescribed classes of graphs.
The Relationships Between Wiener Index, Stability Number and Clique Number of Composite Graphs

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²Department of Mathematical Science, Sharif University of Technology, Tehran, 11365-9415, I. R. Iran
³Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran

Abstract. Some new relations have been established between Wiener indices, stability numbers and clique numbers for several classes of composite graphs that arise via graph products.

Keywords: Wiener index, stability number, clique number, composite graph, product graph

References


Eccentric Connectivity Index of Composite Graphs

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10000 Zagreb, CROATIA

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Abstract. We present explicit formulae for the values of eccentric connectivity index for several families of composite graphs. The results are applied to some graphs of chemical interest, such as C₄ nanotubes and nanotori.

Keywords: eccentric connectivity index, product graph, composite graph
Fractal Patterns In Fullerene Graphs

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Department of Computer Engineering, The University of Kashan

Abstract. Fractals are popular because of their ability to create complex images using only several simple parameters. This is possible by capturing image redundancy and presenting the image in compressed form using the self similarity feature of fractals. A fullerene graph is a planar cubic 3-connected graph. In this research, the novel concept of using fractal pattern to describe the structure of some fullerene graphs is presented.
Dependence Of Lipid Membranes On Changes in Thermodynamic Variables

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Abstract. Biological membranes display complex compositions with hundreds of different lipids and proteins. Our research has shown that the lipid composition varies between different cells and even between different organelles of the same cell. They are also distributed differently between the two monolayers. We have also found that the lipid composition changes as a function of growth conditions, i.e., if ambient temperature, pressure, or the polarity of the aqueous medium are changed. Most lipids in biological membranes are phospholipids with glycerol backbone that possess a phosphate-containing head group and two hydrocarbon chains. Lipid head groups differ in their net charge, their size, and their polarity. Lipid chains differ in length and the degree of unsaturation, i.e., in the number of double bonds. Lipid chains are apolar. The lipid composition of different biological membranes is specific for different cell types and even for the different organelles within one cell and it varies considerably. This is true for both head group composition and the chain composition. Seemingly, the lipid composition responds to changes in intensive thermodynamic variables such as temperature, pressure, pH, or the concentration of solvents. The reason for this is not completely clear.

Furthermore the lipid composition of bio membranes responds sensitively to changes in temperature and pressure. For example trout raised at two different temperatures, 5°C and 20°C. The lipid composition of trout livers changes with growth temperature. The data show that saturated chains are more abundant in trout livers from the 20°C
experiment, while the poly-unsaturated chains are more abundant in the 50°C experiments. Lipid membranes display melting transitions. Such transitions depend on the chain length and the degree of saturation (i.e., the number of double bonds in the chain). The longer the chains the higher the melting point. However, double bonds in a chain drastically lower the melting temperature. DOPC (dioleoyl-phosphatidylcholine) has a melting temperature around -20°C while DSPC (distearoyl-phosphatidylcholine) has a melting temperature of about 53°C. The only difference between these lipids is a double bond between carbons 9 and 10 in the chains of DOPC. It is assumed that many biological phenomena can be understood on the basis of such transitions-including nerve pulse propagation, anesthesia, and membrane permeability. Phase transitions in membranes depend on more variables than just temperature. Among those are also pressure, pH, and the chemical potentials of ions such as Ca²+. Pressure, as an example, shifts melting temperatures towards higher temperatures. Changes in pressure change the physical state of lipid membranes and it seems likely that the membranes of the organisms have to adapt to pressure changes. The pressure dependence of lipid membrane states is not very pronounced and it needs relatively high pressures to see reasonable changes. Typically, 40 bar of pressure changes melting transitions by about 10 K. Therefore, to see similar changes of 150 K temperature difference one requires about 600 bars.

Pressure and temperature are not the only intensive variables in thermodynamics. There are also other variables such as the electrostatic potential, and the chemical potentials of all components of the biological systems. The presence of ethanol lowers melting temperatures. Therefore ethanol should result in a similar change in lipid composition to those caused by temperature increase. We have found that both head group and chain composition are affected. It is likely that changes in other thermodynamic variables will result in comparable changes. The lowering of ambient pH is expected to result in changes similar to those of pressure increase. This is because a certain fraction of the lipids are negatively charged and can be protonated. Protonation of charged lipids increases their melting temperature.
The Wiener Polarity Index of Some Graph Operations

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Abstract. The molecular graph of a molecule \( M \) is a graph which has atoms of \( M \) as vertices and two atoms are adjacent if there is a bond between them. A topological index is a number related to a molecular graph invariant under automorphisms of \( G \). The Wiener polarity index \( W_p(G) \) of a graph \( G \) is defined the number of unordered pairs of vertices \( u \) and \( v \) of \( G \) such that the distance \( d_G(u,v) = 3 \). In this paper this topological index under some graph operations are studied.

Keywords: Wiener polarity index; graph operation
Hosoya and Merrifield-Simmons indices and Their properties

Khadije Fathalikhani* and Hasan Yousefi-Azari**

Abstract. The Hosoya index or z-index of a graph G is the total number of its matchings plus one; the one corresponds to a matching in a set with zero edges. The Merrifield-Simmons index of G, denoted by i(G), is defined as the total number of independent sets of G. These two indices are the prominent examples of topological indices which are of interest in combinatorial chemistry. The z-index was introduced by Hosoya in 1971 and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physicochemical properties such as boiling point, entropy or heat of vaporization are well studied.

Similar connections are known for the i-index, introduced by Merrifield and Simmons in 1989. For detailed information on the chemical applications, we refer to [4].

In this paper, the Hosoya index of a special group of trees, called caterpillars, is calculated. In addition, we have found a lower bound for the i-index of k-colorable graphs. Furthermore, a relation between i-indices of two graph functions is gained.

Key words: Hosoya index, Merrifield-Simmons index, k-colorable graph

References.


3. J.A. Bundy, U.S.R Murty, Graph theory with applications, the Macmillan Press Ltd, Great Britain (1976)

4. R.E. Merrifield and H.E. Simmons, Topological methods in chemistry, Wiley, New York (1989) Speaker (No.4, Koohrang Shaghi Street, Gol Ara Street, AmirKabir Bl, Dehkade Olampic BL, Tehran, Iran. (fathalikhani.kh@gmail.com)**School of mathematics, Statistics and Computer Science, University of Tehran, (hyousefi@ut.ac.ir)
Some Bounds On The General Atom-Bond Connectivity Index Of a Graph

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Abstract. Let G be a simple graph and E(G) be the edge set of G. The general Atom-Bond connectivity index of a Graph G is defined as:

\[ ABC_{\text{general}}(G) = \sum_{\{u,v\} \in E(G)} \sqrt{Q_u + Q_v - 2} \frac{1}{Q_uQ_v}. \]

Some upper and lower bounds for the General Atom-Bond Connectivity Index of a Graph are presented.

Keywords: General atom-bond connectivity index, Randic index.

References


Computation of the Number of Closed Walks In Two Types of
Nanostars Dendrimers

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Abstract. Let G=(V,E) be a graph. A sequence v0v1…vtv0 of vertices of a graph G is called a closed walk if vtv0 , vivi+1 are in E(G), 0 \leq i \leq t – 1. In this paper, the number of closed walks of length k, CW(G, k), for two types of Nano stars are computed, where k is a positive integer.

Keywords: Nano star, closed walk.

References

QSPR Analysis Of Phenolic Antioxidants Using Artificial Neural Network

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1. Introduction

Phenolic antioxidants have an important role in scavenging free radicals, which can damage membranes, proteins, enzymes and DNA [1]. These radicals play an important role in the initiation and promotion of various diseases such as cancer, Alzheimer's, Parkinson's, arthritis, asthma and diabetes. There are many reports in the literature, which elucidate quantitative structure-property relationship (QSPR) of antioxidant using O-H bond dissociation, ionization potential, etc. [2]. Nevertheless, only a few investigations have been done on redox potential. In present work, a QSPR method was developed and applied to predict redox potential of 42 phenolic antioxidants by using artificial neural network (ANN). This developed ANN model can be use to estimate the redox potentials or antioxidant activities of new phenolic compounds by QSPR approaches. To the best of our knowledge, this is the first ANN model, which constructed on this dataset.

2. Experimental

2.1. Data set

The data set in this investigation was taken from paper repoted by Reis et al. [3]. The name of compounds in data set, corresponding observed and ANN predicted redox
potential values at pH=7 (E\textsubscript{7}) are shown in Table 1. This data set is divided into training, internal and external test sets, which used to training network, avoid over-fitting and validation of model, respectively.

### 2.2. Molecular Descriptors

All structures of molecules were drawn with Hyperchem (ver. 7.0) program and optimized by the Am1 semi-empirical method. The drawn molecules exported in a file format suitable for MOPAC (ver. 6.0) package. MOPAC output files were used by CODESSA program to calculate constitutional, topological, geometrical, electrostatic and quantum-chemical descriptors. In addition, Hyperchem output files were used by DRAGON (ver. 3.0) package to calculate topological descriptors. Then the most relevant descriptors selected by stepwise multiple linear regression (MLR) method. This descriptors are: HOMA (Harmonic Oscillator Model of Aromaticity) index, nOH (number of hydroxyl groups) and HOMO (Highest Occupied Molecular Orbital) energy. These descriptors were used as inputs to generate ANN model.

**Table 1.** The data set and corresponding experimental and ANN predicted values of the redox potential at pH=7.0 (E\textsubscript{7/(V)})

<table>
<thead>
<tr>
<th>No.</th>
<th>Name</th>
<th>E\textsubscript{7exp}</th>
<th>E\textsubscript{7cal}</th>
<th>No.</th>
<th>Name</th>
<th>E\textsubscript{7exp}</th>
<th>E\textsubscript{7cal}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4-O\textsubscript{2}NphOH</td>
<td>1.23</td>
<td>1.21</td>
<td>22</td>
<td>2,6-(H\textsubscript{2}C\textsubscript{2})phOH</td>
<td>0.77</td>
<td>0.84</td>
</tr>
<tr>
<td>2</td>
<td>4-NCphOH</td>
<td>1.17</td>
<td>1.10</td>
<td>23</td>
<td>2-H\textsubscript{2}CO, 4-H\textsubscript{2}CphOH</td>
<td>0.68</td>
<td>0.69</td>
</tr>
<tr>
<td>3</td>
<td>3,5-CIphOH</td>
<td>1.15</td>
<td>1.10</td>
<td>24</td>
<td>3,4-(H\textsubscript{2}CO)phOH</td>
<td>0.67</td>
<td>0.67</td>
</tr>
<tr>
<td>4</td>
<td>4-F\textsubscript{2}CphOH</td>
<td>1.13</td>
<td>1.17</td>
<td>25</td>
<td>3,4,5-(H\textsubscript{2}CO)\textsubscript{3}phOH</td>
<td>0.66</td>
<td>0.57</td>
</tr>
<tr>
<td>5</td>
<td>4-phiOCphOH</td>
<td>1.12</td>
<td>1.04</td>
<td>26</td>
<td>2-HO, 4-HOOCphOH</td>
<td>0.60</td>
<td>0.65</td>
</tr>
<tr>
<td>6</td>
<td>3-NCphOH</td>
<td>1.11</td>
<td>1.13</td>
<td>27</td>
<td>2,6-(H\textsubscript{2}CO)\textsubscript{3}phOH</td>
<td>0.58</td>
<td>0.54</td>
</tr>
<tr>
<td>7</td>
<td>4-phiOH</td>
<td>1.09</td>
<td>1.02</td>
<td>28</td>
<td>2,3-(HO)\textsubscript{2}phOH</td>
<td>0.58</td>
<td>0.53</td>
</tr>
<tr>
<td>8</td>
<td>4-HOOCphOH</td>
<td>1.04</td>
<td>1.00</td>
<td>29</td>
<td>3,4-Dihydroxynamic acid</td>
<td>0.54</td>
<td>0.53</td>
</tr>
<tr>
<td>9</td>
<td>3-H\textsubscript{2}COphOH</td>
<td>0.98</td>
<td>1.08</td>
<td>30</td>
<td>2-HOphOH</td>
<td>0.53</td>
<td>0.62</td>
</tr>
<tr>
<td>10</td>
<td>4-H\textsubscript{2}CphOH</td>
<td>0.97</td>
<td>0.96</td>
<td>31</td>
<td>2-HO, 4-H\textsubscript{2}CphOH</td>
<td>0.52</td>
<td>0.58</td>
</tr>
<tr>
<td>11</td>
<td>4-phiCphOH</td>
<td>0.94</td>
<td>0.96</td>
<td>32</td>
<td>2-HO, 4-H\textsubscript{2}CphOH</td>
<td>0.41</td>
<td>0.39</td>
</tr>
<tr>
<td>12</td>
<td>4-FphOH</td>
<td>0.93</td>
<td>0.91</td>
<td>33</td>
<td>3-O\textsubscript{2}NphOH</td>
<td>1.13</td>
<td>1.21</td>
</tr>
<tr>
<td>13</td>
<td>Tyrosine</td>
<td>0.89</td>
<td>0.79</td>
<td>34</td>
<td>4-BphOH</td>
<td>0.96</td>
<td>0.98</td>
</tr>
<tr>
<td>14</td>
<td>4-H\textsubscript{2}CphOH</td>
<td>0.87</td>
<td>0.85</td>
<td>35</td>
<td>3-HO, 5-H\textsubscript{2}CphOH</td>
<td>0.84</td>
<td>0.76</td>
</tr>
<tr>
<td>15</td>
<td>3,5-(H\textsubscript{2}CO)\textsubscript{3}phOH</td>
<td>0.85</td>
<td>0.84</td>
<td>36</td>
<td>4-H\textsubscript{2}CphOH</td>
<td>0.73</td>
<td>0.74</td>
</tr>
<tr>
<td>16</td>
<td>3-H\textsubscript{2}CphOH</td>
<td>0.85</td>
<td>0.90</td>
<td>37</td>
<td>2,3-(HO)\textsubscript{2}, 5-H\textsubscript{2}COOCphOH</td>
<td>0.56</td>
<td>0.61</td>
</tr>
<tr>
<td>17</td>
<td>3,5-(H\textsubscript{2}CO)\textsubscript{3}phOH</td>
<td>0.84</td>
<td>0.89</td>
<td>38</td>
<td>4-H\textsubscript{2}COCphOH</td>
<td>1.06</td>
<td>1.07</td>
</tr>
<tr>
<td>18</td>
<td>4-phiCphOH</td>
<td>0.84</td>
<td>0.71</td>
<td>39</td>
<td>3-HO, 4-H\textsubscript{2}COCphOH</td>
<td>0.89</td>
<td>0.86</td>
</tr>
<tr>
<td>19</td>
<td>2-H\textsubscript{2}CphOH</td>
<td>0.82</td>
<td>0.89</td>
<td>40</td>
<td>3-HOphOH</td>
<td>0.81</td>
<td>0.81</td>
</tr>
<tr>
<td>20</td>
<td>4-tert-butylphiOH</td>
<td>0.80</td>
<td>0.86</td>
<td>41</td>
<td>Sesamol</td>
<td>0.62</td>
<td>0.65</td>
</tr>
<tr>
<td>21</td>
<td>2-H\textsubscript{2}COCphOH</td>
<td>0.77</td>
<td>0.73</td>
<td>42</td>
<td>4-HOOCphOH</td>
<td>0.46</td>
<td>0.62</td>
</tr>
</tbody>
</table>
In the above table, compounds 33-37 and 38-42 constitute the external and internal test sets, respectively.

3. Result and discussion

The ANN model was constructed using statistica neural networks (SNNs) (ver. 7.0). Among many types of ANN, Multilayer perceptron was applied. We used a two-phase algorithm namely, back-propagation and levenberg-marquardt for training the network. The ANN inputs are three molecular descriptors, which were selected by stepwise MLR method, while its output signal represents the redox potential of interested molecules. The number of nodes in hidden layer, learning rate and momentum has been optimized before training the network. Table 2 shows the architecture and specification of the optimized network. The root mean square error in prediction of $E_7$ for training, internal and external test sets are: 0.048, 0.050 and 0.051 respectively. Other statistical parameters obtained from this model are shown in table 3. These results reveal the robustness and capability of ANN based on QSPR model in prediction of redox potential of various antioxidants. Fig. 1 shows the plot of ANN calculated versus experimental values of redox potential. A good correlation for this plot confirms the ability of the ANN model in prediction of redox potential. The residuals of ANN calculated values of redox potential plotted against their experimental values in Fig. 2. The propagation of the residuals on both sides of zero line indicates that there isn't any systematic error in the developed ANN model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nodes in the input layer</td>
<td>3</td>
</tr>
<tr>
<td>Number of nodes in the hidden layer</td>
<td>4</td>
</tr>
<tr>
<td>Number of nodes in the output layer</td>
<td>1</td>
</tr>
<tr>
<td>Learning rate</td>
<td>0.4</td>
</tr>
<tr>
<td>Momentum</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 3. Statistical parameters obtained using the ANN model.

<table>
<thead>
<tr>
<th>Set</th>
<th>$R$</th>
<th>SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training</td>
<td>0.968</td>
<td>0.047</td>
</tr>
<tr>
<td>Internal</td>
<td>0.961</td>
<td>0.057</td>
</tr>
<tr>
<td>External</td>
<td>0.957</td>
<td>0.066</td>
</tr>
</tbody>
</table>
**Keywords:** Quantitative structure-property relationship, Phenolic antioxidant, Artificial neural network

**References:**

Eccentric Connectivity Polynomial of an Infinite Family of Fullerenes

M. Ghasemi, M. Ghorbani and A. Azad

Abstract. The eccentric connectivity index of molecular graph $G$, $\zeta^e(G)$, was proposed by Sharma, Goswami and Madan. It is defined as $\zeta^e(G) = \sum_{u \in V(G)} \text{deg}_G(u) \text{ecc}(u)$, where $\text{deg}_G(x)$ denotes the degree of vertex $x$ in $G$ and $\text{ecc}(u) = \text{Max}\{d(x, u) \mid x \in V(G)\}$.

The eccentricity connectivity polynomial of a molecular graph $G$ defined as

$ECP(G, x) = \sum_{a \in V(G)} \text{deg}_G(a)x^{\text{ecc}(a)}$ where $\text{ecc}(a)$ is defined as the length of a maximal path connecting $a$ to another vertex of $G$. In this paper this polynomial is computed for triangular benzenoid graphs.

Keywords: Eccentric connectivity index

References


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Srtt University, Tehran, Iran, October 6-7, 2010

The Enumeration Of IPR Hetero-Fullerenes Constructed By Leapfrog Principle

M. Ghazi and S. Shakeraneh

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Abstract. Hetero-fullerenes are fullerene molecules in which one or more carbon atoms are replaced by hetero-atoms such as boron or nitrogen, whose formation is a kind of “on-ball” doping of the fullerene cage. In this paper by using the Pólya’s theorem we compute the number of possible positional isomers and chiral isomers of the hetero-fullerenes.

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Keywords: Fullerene, Hetero-fullerene, Leapfrog Principle, Cycle Index.

Reference


Computing Omega and PI Polynomials of Graphs

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Abstract. A new counting polynomial, called Omega $\Omega(G,x)$, was recently proposed by Diudea. It is defined on the ground of “opposite edge strips” ops. The Sadhana polynomial $Sd(G,x)$ can also be calculated by ops counting. In this paper we compute these polynomials for some classes of 8 – cycle graphs.

Key words: Omega polynomial, Sadhana Polynomial, 8 -Cycles Graph.

References
Omega polynomial of Polyomino Chains

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Abstract. A new counting polynomial, called Omega $\Omega(G,x)$, was recently proposed by Diudea. It is defined on the ground of “opposite edge strips” ops. The Sadhana polynomial $Sd(G,x)$ can also be calculated by ops counting. In this paper we compute these polynomials for 4–cycles graph.

Key words: Omega polynomial, Sadhana Polynomial, 8 -Cycles Graph.

Reference

On The Wiener and Szeged Indices of Some Nano Structures

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Abstract. An important invariant of connected graphs is the Wiener index, which is equal to the sum of distances between all pairs of vertices of the respective graph. In this paper by using a new method introduced by klavzar we compute the Wiener and Szeged indices of some partial cube graphs.

Key words: Wiener index, Szeged index, Polyomino Chains, Triangular Benzenoid

Reference

Computing $ABC$ Index of Nanostar Dendrimers

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Abstract. The $ABC$ index is a topological index was defined as

$$ABC(G) = \sum_{u \neq v} \frac{d(u) + d(v) - 2}{d(u)d(v)},$$

where $d(u)$ denotes degree of vertex $u$. In this paper we compute this new topological index for $C_4C_8$ nanotubes.

Key words: Topological Index, $ABC$ Index, Nanotubes.

References


Hosoya Polynomials Of \( TUC_4C_8(R) \) Nanotours

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Abstract. In the fields of chemical graph theory and in mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure.

The Hosoya polynomial of a connected graph \( G \), denoted by \( H(G, x) \) and is defined as:

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

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 [1,2], especially two well-known topological indices, i.e.; Wiener index and hyper-Wiener index, can be directly obtained from this polynomial.

The Wiener index of a connected graph \( G \), \( W(G) \) is equal to the sum of distances between all pairs of vertices in \( G \) [3]. That is

\[
W(G) = \sum_{(u,v) \in V(G)} d(u,v)
\]

The hyper-Wiener index of graph \( G \), \( WW(G) \) is defined as [4]:
From Eqs (1) and (2) the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index, i.e;

$$W(G) = H'(G,x)|_{x = 1} \quad (4)$$

Also, from Eqs (1,3) the following relation holds:

$$WW(G) = \frac{1}{2} \left( xH(G,x) \right)^{\prime \prime} |_{x = 1} \quad (5)$$

We described TUC$_4$C$_8$(R) nanotorus by two parameters $p$ and $q$ and simply denoted by $T[p,q]$ which $p$ is the number of rhombs on the level 1 and the length of torus is $q$.

The main result of this paper, is the following theorem:

**Theorem:** If $1 \leq q \leq \left[ \frac{p+4}{2} \right]$, then:

$$H(p,q,x) = \frac{pq}{(x^2-1)(x-1)} \left( 1+x \right) \left( 3x^2+2x+2 \right) - x^{2q-1}(x-1)(x^2+x+2)-2(1+x^2)(1+x)n^{2q}+1(1+x^2) \left( 1-x \right)^{\frac{q}{2}} \left( \frac{2x+1}{x-1} \right)$$

where $a = \left[ \frac{p+1}{2} \right], \quad \pi_p = \begin{cases} 0, & \text{if } p \text{ is odd} \\ 1, & \text{if } p \text{ is even} \end{cases}$.

**Keywords:** Hosoya polynomial, Wiener index, hyper-Wiener index, TUC$_4$C$_8$(R) nanotorus.
References


Computing Eccentric Connectivity Polynomial Of Fullerenes

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Department of Mathematics, Faculty of Science, Yazd University, Yazd, I. R. Iran

Abstract The eccentricity connectivity polynomial of a molecular graph G is defined as
\[ \xi(x) = \sum_{a \in V(G)} x^{\varepsilon(a)}, \]
where \( \varepsilon(a) \) is defined as the length of a maximal path connecting a to another vertex of G. Fullerenes are 3 cubic graphs with exactly 12 pentagonal faces. In this paper this polynomial is computed for an infinite family of fullerenes.

Keywords: Eccentricity Connectivity Polynomial, Eccentricity Connectivity Index, Fullerene Graphs.

References


On Omega and Sadhana Polynomials Of Leapfrog Fullerenes $F_{36c3}^l$

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Abstract. A leapfrog transform $G^l$ of $G$ is a graph on $3n$ vertices obtained by truncating the dual of $G$. Hence, $G^l = Tr(G^*)$, where $G^*$ denotes the dual of $G$. It is easy to check that $G^l$ itself is a fullerene graph. In this paper, the Omega and Sadhana polynomials of a new infinite class of Leapfrog fullerenes are computed for the first time.

Key words: Omega Polynomial, Sadhana Polynomial, Fullerene Graph, Leapfrog Fullerene.

References


Y-Wiener Index of Composite Graphs

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Abstract. Eliasi and Taeri [Extension of the Wiener index and Wiener polynomial, Appl, Math. Lett. 21 (2008), 916-921.] introduced the notion of y-Wienerindex of graphs as a gegeralization of the classical Wiener index and hyperWiener index of graphs. They obtained some mathematical properties ofthis new defined topological index. In this paper, the join, Cartesian Product,composition, disjunction and symmetric difference of graphs under y-Wienerindex are computed. By these results most part of a paper by Sagan et al and another paper by Khalifeh et al are generalized.

Keywords: y-Wiener index, Cartesian Product, join

Introduction

Suppose G is a simple connected graph. As usual, the distance between the vertices \( u \) and \( v \) of G is denoted as \( d_G(u,v) \). It is defined as the length of a minimum path connecting them. The maximum of such number, \( \text{diam}(G) \), is said to be the diameter of G.
The number of pairs of vertices of $G$ that are at distance $k$ is denoted by $d(G,k)$. Notice that $d(G,0)$ and $d(G,1)$ represent the number of vertices and edges of $G$, respectively.

A topological index is a number related to a graph invariant under isomorphism. Obviously, the number of vertices and edges of a given $G$ are topological indices of $G$. The Wiener index is the first distance based topological index defined by chemist Harold Wiener. This index is defined as the sum of all distances between vertices of $G$. After Wiener, too many authors continued the pioneering work of Wiener by introducing new topological index.

The join $G + H$ of disjoint graphs $G$ and $H$ is the graph obtained from $G \cup H$ by joining each vertex of $G$ to each vertex of $H$. The Cartesian product $G \times H$ of graphs $G$ and $H$ has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$ or $ab \in E(G)$ and $x = y$.

The composition $G = G_1[G_2]$ of graphs $G_1$ and $G_2$ with disjoint vertex sets $V_1$ and $V_2$ and edge sets $E_1$ and $E_2$ is the graph with vertex set $V_1 \times V_2$ and $u = (u_1,v_1)$ is adjacent with $v = (u_2,v_2)$ whenever $(u_1$ is adjacent with $u_2)$ or $(u_1 = u_2$ and $v_1$ is adjacent with $v_2$).

The disjunction $G \vee H$ of graphs $G$ and $H$ is the graph with vertex set $V(G) \times V(H)$ and $(u_1,v_1)$ is adjacent with $(u_2,v_2)$ whenever $u_1u_2 \in E(G)$ or $v_1v_2 \in E(H)$. The symmetric difference $G \oplus H$ of two graphs $G$ and $H$ is the graph with vertex set $V(G) \times V(H)$ and $E(G \oplus H) = \{(u_1,u_2)(v_1,v_2) \mid u_1v_1 \in E(G) \text{ or } u_2v_2 \in E(H) \text{ but not both}\}$.

The Gamma function is a generalization of the well-known factorial function. It is defined as $\Gamma(x) = \int_0^\infty t^{x-1}e^{-t}dt$. Remember that the Gamma function has the following properties: (i) $\Gamma(x+1) = x\Gamma(x)$, and, (ii) if $k$ is a non-negative integer then $\Gamma(k+1) = k!$.

We now assume that $y$ is a positive real number and $G$ be a graph. Then $W(G,y)$, the $y$-Wiener index of $G$, is defined as $W(G,y) = \sum_{(u,v) \in V(G)} \frac{\Gamma(d_G(u,v)+y)}{y\Gamma(d_G(u,v))}$. It is easy to see that this definition is equivalent to
\[ W(G,y) = \sum_{i=1}^{l} \frac{\Gamma(t+y)}{y\Gamma(t)} d(G,t), \]
where \( l \) denotes the diameter of \( G \). One can see that \( W(G,1) \) is classical Wiener index and \( W(G,2) \) is well-known hyper-Wiener index of \( G \).

**Main Results**

**Theorem 1:** Let \( G \) and \( H \) be connected graphs and \( l = \text{diam}(G) + \text{diam}(H) \). Then

\[ W(G \times H, y) = |V(H)| W(G, y) + 2 \sum_{i=1}^{l} \frac{\Gamma(t+y)}{y\Gamma(t)} \sum_{i=1}^{l} d(G,i)d(H,t - 1). \]

**Theorem 2:** Let \( G \) and \( H \) be connected graphs. Then

\[ W(G + H, y) = \Gamma(y) \left( \frac{|V(G)|(|V(G)| - 1)}{2} + \frac{|V(H)|(|V(H)| - 1)}{2} + |V(G) \parallel V(H)| \right) \]

\[ + y\Gamma(y)(|E(G)| + |E(H)|). \]

**Theorem 3:** Let \( G \) and \( H \) be connected graphs. Then

\[ W(G \vee H, y) = \Gamma(y)(|E(G) \parallel V(H)|^2 + |E(H) \parallel V(G)|^2 - 2|E(G) \parallel E(H)|) \]

\[ + (y + 1)\Gamma(y)(|E(G) \parallel E(H)| + |V(H) \parallel E(G)| + 2|E(G) \parallel E(H)|). \]

**Theorem 4:** Let \( G \) and \( H \) be connected graphs. Then

\[ W(G \otimes H, y) = \Gamma(y)(|E(G) \parallel V(H)|^2 + |E(H) \parallel V(G)|^2 - 4|E(G) \parallel E(H)|) \]

\[ + (y + 1)\Gamma(y)(2|E(G) \parallel E(H)| + |V(G) \parallel E(H)|). \]
Theorem 5: Let G and H be connected graphs. Then

\[ W(G[H], y) = \Gamma(y) |V(G)| \frac{|V(H)|(|V(H)| - 1)}{|V(H)|} + y\Gamma(y)|E(H)||V(G)| + |V(H)|^2 W(G, y). \]

References


Eccentric Connectivity Polynomial Of $C_{12(2n+1)}$ Fullerenes

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Abstract. Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. If $x, y \in V(G)$ then the distance $d(x, y)$ between $x$ and $y$ is defined as the length of a minimum path connecting $x$ and $y$. The eccentric connectivity index of the molecular graph $G$, $\xi_c(G)$, was proposed by Sharma, Goswami and Madan. It is defined as $\xi_c(G) = \sum_{u \in V(G)} \text{deg}_G(u) \text{ecc}(u)$, where $\text{deg}_G(x)$ denotes the degree of the vertex $x$ in $G$ and $\text{ecc}(u) = \max\{d(x, u) \mid x \in V(G)\}$ . The radius and diameter of $G$ are defined as the minimum and maximum eccentricity among vertices of $G$, respectively. We now define the eccentric connectivity polynomial of a graph $G$, $ECP(G, x)$, as $ECP(G, x) = \sum_{a \in V(G)} \text{deg}_G(a) x^{\text{ecc}(a)}$ and then calculate the second derivative of $ECP(G, x)$ evaluated at $x = 1$. 
Extremal Properties Of Zagreb Coincides and Degree Distance Of Graphs

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Abstract: The degree distance and Zagreb coinindices of a connected graph, has been studied in mathematical chemistry. In this paper some new extremal values of these topological invariants over some special classes of graphs are determined.

Keywords: degree-distance, Zagreb index, Zagreb coindex, reverse degree distance.

Introduction

All graphs in this paper are finite and simple. A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are also called topological indices. Among graph invariants two that are known under various names, but mostly as Zagreb indices. Let \( G \) be a connected graph with vertex and edge sets \( V(G) \) and \( E(G) \), respectively. For every vertex \( u \in V(G) \) the edge connecting \( u \) and \( v \) is denoted by \( uv \) and \( \deg_G(u) \) denotes the degree of \( u \) in \( G \). The distance \( d_G(u, v) \) is defined as the length of a minimum path connecting \( u \) and \( v \) and the diameter of \( G \), \( \text{diam}_G(G) \), is the maximum possible distance between any two vertices in the graph. We will omit the subscript \( G \) when the graph is clear from the context. The first and second Zagreb indices were originally defined as \( M_1(G) = \sum_{u \in V(G)} \deg_G(u)^2 \) and \( M_2(G) = \sum_{uv \in E(G)} \deg_G(u)\deg_G(v) \), respectively.
The first Zagreb index can be also expressed as a sum over edges of G, $M_1(G) = \sum_{uv \in E(G)} [\deg_G(u) + \deg_G(v)]$.

The first and second Zagreb coindices was first introduced by Došlić. They are defined as $\overline{M}_1(G) = \sum_{uv \notin E(G)} [\deg_G(u) + \deg_G(v)]$ and $\overline{M}_2(G) = \sum_{uv \notin E(G)} \deg_G(u)\deg_G(v)$.

In some recent papers Dobrynin and Kochetova and Gutman introduced a new graph invariant defined as:

$$D'(G) = \sum_{x \in V(G)} D'(x) = \sum_{x \in V(G)} D(x)\deg_G(x) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y) [\deg_G(x) + \deg_G(y)]$$

where $D'(x) = D(x)\deg_G(x)$, $\deg_G(x)$ is the degree of $x$ and $D(x) = \sum_{y \in V(G)} d_G(x,y)$.

If $G$ is $n$-vertex graph then the reverse Wiener matrix is an $n \times n$ matrix $RW(G) = [RW_{ij}]$ such that $RW_{ij} = diam(G) - d(v_i,v_j)$, if $i \neq j$ and $0$ otherwise. The reverse degree distance of $G$ is defined as $D(G) = \sum_{i=1}^{n} \deg_G(v_i) \sum_{j=1}^{n} RW_{ij}$.

The girth of $G$ is the length of a shortest cycle contained in $G$. A Moore graph is a graph of diameter $k$ with girth $2k + 1$. Those graphs have the minimum number of vertices possible for a regular graph with given diameter and maximum degree. For $k$ a real number, let $\sum_k(G)$ denote the sum of the $k$-th powers of the degrees of $G$. We denote by $\sigma_2(n,m)$ the maximum value of $\sum_k(G)$ when $G$ is a graph (not necessarily connected) with $n$ vertices and $m$ edges. Also, let $\sum_k(n,m) = \max_{G \in \rho_{n,m}}$ that $\rho_{n,m}$ denote the family of connected graphs on $n$ vertices and $m$ edges.

The subdivision graph $S(G)$ of a graph $G$ is obtained by inserting a new vertex of degree two on each edge of $G$. If $G$ has $n$ vertices and $m$ edges, then $S(G)$ has $n + m$ vertices and...
2m edges. The join \( G+H \) of graphs \( G \) and \( H \) with disjoint vertex sets \( V(G) \) and \( V(H) \) and edge sets \( E(G) \) and \( E(H) \) is the graph union \( G \cup H \) together with all the edges joining \( V(G) \) and \( V(H) \).

2. Main Result

In this section some new extremal values of Zagreb coindices, degree distance and reverse degree distance over some special classes of graphs are determined. Let \( G \) be a connected graph with minimal degree \( \delta \) and maximal degree \( \Delta \).

Proposition 1. Let \( G \) be a simple graph with \( n \) vertices, \( m \) edges. Then

\[
M_1(G) \leq \frac{-4m^2}{n} + 2m(n-1) \text{ with equality if and only if } G \text{ is regular.}
\]

Proposition 2. Let \( G \) be a simple graph with \( n \) vertices, \( m \) edges. Then

\[
2m^2 - \frac{M_1(G)}{2} (\Delta + 1) \leq M_2(G) \leq 2m^2 \left(1 - \frac{2m}{n} - \frac{1}{n}\right). \text{ The right hand (left hand) side of this inequality is satisfied if and only if } G \text{ is regular.}
\]

Proposition 3. Let \( G \) be a simple graph with \( n \) vertices, \( m \) edges. Then

(a) \( M_1(S(G)) \leq 4m(n-2) + 4m^2 \left(1 - \frac{1}{n}\right), \text{ the equality holds if and only if } G \text{ is regular.}\)

(b) \( M_2(S(G)) \leq 8m^2 - 2m - \frac{10m^2}{n}, \text{ the equality holds if and only if } G \text{ is regular.}\)

(c) \( M_2(S(G)) = -2m^2 + 18m - 10mn + \frac{5}{2}M_1(S(G)).\)

Proposition 4. Suppose \( G \) is a graph with \( n \) vertices, \( m \) edges. Then

\[
M_1(G) \geq 2m(n-1) - m(\Delta + \delta + 1).
\]
Proposition 5. Suppose $G$ is a connected graph with $n$ vertices, $m$ edges.

$$M_1(G) \geq 2m(n-1) - \frac{(\Delta + \delta)^2}{n\Delta\delta}m^2.$$ The equality holds if and only if $G$ is regular.

Proposition 6. If $G$ is a connected bicyclic graph with $n$ vertices and $m$ edges without pendant vertices, then

$$\frac{M_1(G)}{n} \geq \frac{2m(n-1)}{n} + \frac{M_2(G)}{m} - 2m + \frac{M_1(G)}{2m}$$

with equality if and only if $G$ is isomorphic to $K_{2,3}$.

Proposition 7. Let $G$ be a graph of order $n$ containing $m$ edges, then

$$2(m^2 + \overline{m}^2) - \frac{n(n-1)^3}{2} - \frac{n(n-1)^2}{2} \leq M_2(G) + \overline{M_2(G)} \leq 2(m^2 + \overline{m}^2) - \frac{n(n-1)}{2}\left(\frac{n-1}{2}\right)^2 - \frac{n(n-1)^2}{2}.$$  

The equality in right hand side is satisfied if and only if $n \equiv 1 \pmod{4}$ and $G$ is $\frac{n-1}{2}$-regular. The equality in left hand side is satisfied if and only if $G$ is isomorphic to complete graph $K_n$.

Proposition 8. If $1 \leq n-1 \leq m$ and $G$ is a connected graph with $n$ vertices and $m$ edges, then

$$\mathcal{D}'(G) \leq -4(n-1)m + \sum_{z}(n,m) + 2m(n-1)diam(G).$$

Equality happens if and only if $G$ is a join of $K_1$ and a graph $G'$ on $n-1$ vertices and $m+n-1$ edges with

$$\sum_{z}(G') = \sigma_z(n-1,m-n+1).$$

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References


A New Polynomial Of Some Graph Operations

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Abstract. The eccentric connectivity index of the molecular graph $G$, $\xi_c(G)$, was proposed by Sharma, Goswami and Madan. It is defined as $\xi_c(G) = \sum_{u \in V(G)} \deg_G(u)e_G(u)$, where $\deg_G(x)$ denotes the degree of the vertex $x$ in $G$ and $e_G(u) = \max\{d(x, u) | x \in V(G)\}$. We define the eccentric connectivity polynomial of a graph $G$, $\xi_c(G, x)$, as $\xi_c(G, x) = \sum_{a \in V(G)} \deg_G(a)x^{e_G(a)}$. Then the eccentric connectivity index is the first derivative of $ECP(G, x)$ evaluated at $x = 1$. In this paper we compute this new polynomial for some graph operations.

Keywords: Graph Operations, Topological Index, Eccentric Connectivity Polynomial.

References


Computing $ABC_4$ Index of Nanostar Dendrimers

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Abstract. The $ABC$ index is a topological index was defined as $ABC(G) = \sum_{u \in V(G)} \sqrt{d_u(u) + d_u(v) - 2 \over d_u(u)d_v(v)}$, where $d_u(u)$ denotes degree of vertex $u$. Now we define a new version of $ABC$ index as $ABC_4(G) = \sum_{u \in V(G) \cap E(G)} \sqrt{\delta_u(u) + \delta_v(v) - 2 \over \delta_u(u)\delta_v(v)}$, where $\delta_u(u) = \sum_{v \in E(G)} d_v(v)$. The goal of this paper is to further the study of the $ABC_4$ index.

Key words: $ABC_4$ Index, Nanostar Dendrimers, chemical graph theory.

References


The Eccentric Connectivity Index of Some Special Graphs

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Abstract. If \( G \) is a connected graph with vertex set \( V \), then the eccentric connectivity index of \( G \), \( \chi^e(G) \), is defined as \( \sum_{v \in V} \deg(v) \text{ecc}(v) \) where \( \deg(v) \) is the degree of a vertex \( v \) and \( \text{ecc}(v) \) is its eccentricity. Let A, B and C are families of graphs made by joining \( K_{m,n} \) to \( K_{m,n} \), made by putting \( \overline{K_{m,n}} \) instead of each vertex in \( K_{m,n} \) and made by putting \( \overline{C_{m,n}} \) instead of each vertex in \( K_{m,n} \), respectively. In this paper we compute the eccentric connectivity index of these families of graphs.

Key words: Eccentric Connectivity index, graph.

1. Introduction

A simple graph \( G = (V, E) \) is a finite nonempty set \( V(G) \) of objects called vertices together with a (possibly empty) set \( E(G) \) of unordered pairs of distinct vertices of \( G \) called edges. In chemical graphs, the vertices correspond to the atoms and molecule, and the edges represent the chemical bonds.

If \( x, y \in V(G) \) then the distance \( d(x, y) \) between \( x \) and \( y \) is defined as the graph of a minimum path connecting \( x \) and \( y \). The eccentric connectivity index of the molecular graph \( G = (V, E) \), \( \chi^e(G) \), was proposed by Sharma, Goswami and Madan [3]. It is defined as \( \sum_{v \in V} \deg(v) \text{ecc}(v) \), where \( \deg(v) \) denotes the degree of the vertex \( v \) in \( G \) and \( \text{ecc}(v) = \max [d(v, u) | u \in V(G)] \), see [1,2] for more details.
We denote the complete graph of order \( n \), the cycle of order \( n \) and the path of order \( n \) by \( K_n \), \( C_n \) and \( P_n \), respectively. In section 2 we compute the eccentric connectivity index for some special graphs.

2. The eccentric Connectivity Index Of Some Special Graphs

In this section we compute the eccentric connectivity index of the special graphs \( A \), \( B \) and \( C \) as follows:

a. \( A = \) families of graphs made by joining \( K_m \) to \( P_n \);

b. \( B = \) families of graphs made by putting \( K_m \) instead of each vertex in \( P_n \);

c. \( C = \) families of graphs made by putting \( C_m \) instead of each vertex in \( P_n \).

Note. For a path of order \( n \) we have:

\[
\xi^e(P_n) = \begin{cases} 
\frac{1}{3}(3n^2 - 6n + 4), & \text{if } n \text{ is even} \\
\frac{1}{3}(n - 1)^3, & \text{if } n \text{ is odd}
\end{cases}
\]

**Definition.** Let \( m, n \) are two positive integers. Define \( \alpha_{m,n} \) as

\[
\alpha_{m,n} = (m - 1)^2n + mn(m - 1)
\]

if \( m \) is even, then we define \( \varphi_{m,n} \) as

\[
\varphi_{m,n} = 2\left(\frac{m}{2} + n - 1\right) + 3\max\left(\frac{m}{2}, n - 1\right) + \sum_{j=2}^{m/2} \max\left(\frac{m}{2}, j + n - 2\right)
\]

If \( m \) is odd, then we define \( \psi_{m,n} \) as

\[
\psi_{m,n} = 2\max\left(\frac{m-1}{2}, n - 1\right) + 4\sum_{j=2}^{m/2} \max\left(\frac{m-1}{2}, j + n - 2\right)
\]

**Theorem 1.** Let \( A \), \( B \) and \( C \) are the graphs mentioned. Then the eccentric connectivity indices of these graphs are as follows:

1. \( \xi^e(A) = \xi^e(P_{n+2}) + \alpha_{m(n+1)} - 2(m - 1) \).
2. \[ \xi(B) = \begin{cases} 2(\alpha_{\nu,\nu+1} + \sum_{i=2}^{\nu-1} (\alpha_{\nu,\nu-i} + i - 1)) & \text{if } n \text{ is even} \\ \alpha_{\nu,\nu+1} + \sum_{i=2}^{\nu-1} (\alpha_{\nu,\nu-i} + i - 1) + 2(\alpha_{\nu,\nu+1} + \sum_{i=2}^{\nu-1} (\alpha_{\nu,\nu-i} + i - 1)) & \text{if } n \text{ is odd} \end{cases} \]

3. \[ \xi(C) = \begin{cases} 2\theta_{\nu,\nu+1} + \sum_{i=2}^{\nu-1} \theta_{\nu,\nu-i} + n - \left( \frac{n-1}{2} \right) + \sum_{i=2}^{\nu-1} \theta_{\nu,\nu-i} + n - \left( \frac{n-1}{2} \right) & \text{if } m \text{ is odd} \\ 2\theta_{\nu,\nu+1} + \sum_{i=2}^{\nu-1} \theta_{\nu,\nu-i} + n - \left( \frac{n-1}{2} \right) + \sum_{i=2}^{\nu-1} \theta_{\nu,\nu-i} + n - \left( \frac{n-1}{2} \right) & \text{if } m \text{ is even} \end{cases} \]

References


On Omega Polynomials Of Fullerenes

Mohsen Jaddi

Department of Mathematics, Payame Noor University (PNU), Aran&Bidgol, 87415141, I. R. Iran;

Abstract. A leapfrog transform $G^l$ of $G$ is a graph on $3n$ vertices obtained by truncating the dual of $G$. Hence, $G^l = Tr(G^*)$, where $G^*$ denotes the dual of $G$. It is easy to check that $G^l$ itself is a fullerene graph. In this paper, the Omega and Sadhana polynomials of a new infinite class of Leapfrog fullerenes are computed for the first time.

Key words: Omega Polynomial, Sadhana Polynomial, Fullerene Graph, Leapfrog Fullerene.

References

Computing Omega and Sadhana Polynomials of Fullerenes

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Department of Mathematics, Faculty of Science, Shahid Rajaee
Teacher Training University, Tehran, 16785 – 136, I. R. Iran;

Abstract. The Omega Polynomial at first was introduced by Mircea Diudea. In this paper we compute Omega and Sadhana polynomials of an infinite class of fullerenes.

Key words: Fullerene Graph, Omega Polynomial, Sadhana Polynomial.

References


Counting Polynomials of Some Nanostructures

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Abstract. Fullerenes are 3 regular graphs. Fullerene era was started by discovery of a stable cluster of C\textsubscript{60}. Counting polynomial was introduced by Hosoya. In this paper we compute some counting polynomials of nanostructures.

Key words: Counting Polynomial, Fullerene Graph, Nanostructures.

References


Phase Transitions of Membranes Consisting of One Lipid Species

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Abstract. A membrane represents a two-dimensional matrix embedded into three-dimensional space, which usually consists of an aqueous medium. Lipid membranes display at least two different phases: the solid-ordered phase often called the "gel phase" and the liquid-disordered phase that is often called the "fluid phase. Low temperatures lipids are arranged on a triangular lattice. At high temperatures, they do not display lateral order. Instead, they are randomly organized and represent a liquid in the language of solid state physics. For this reason the transition is called solid-liquid transition. Lipid membranes may undergo order or melting transitions. For biological membranes these transitions are typically found in the range 10-25 °C. Most lipids that are extracted from such membranes melt in the temperature regime between -20\( ^\circ \)C (some lipids with unsaturations in their chains as dioleoyl phosphatidylcholine- DOPC) and +60\( ^\circ \)C (lipids with a long saturated long chain, e.g., some sphingolipids and ceramides). Such melting transitions can be measured with many means, including differential scanning calorimetry (DSC) and various spectroscopic methods. Calorimetry has the advantage that it directly yields important thermodynamic information (e.g., enthalpy and entropy changes) not available (without interpretation) from spectroscopy.

Furthermore, the lipid chains of the individual molecules simultaneously also display order-disorder transitions. Whereas at low temperatures the lipids display predominantly all-trans configurations, at high temperatures they show a rather random chain order with many trans, gauche\(^-\) and gauche\(^+\) isomerisation in their C-C bonds in
the hydrocarbon chain. These terms describe the two different ordering processes in membranes. We have found that the solid-liquid transition of the head group arrangement and the order-disorder transition of the chains do not necessarily have to occur at the same temperature and that possibly solid-disordered and liquid-ordered phases are possible. While the solid-disordered phase has so far not been identified in lipid membranes, the liquid-ordered phase has been proposed to exist in cholesterol-containing membranes, possibly due to the size of the cholesterol molecule that disturbs the formation of lateral lattices and its hydrogen bonding to carbonyl oxygen. The liquid-ordered phase is a kind of gel phase (i.e., with low enthalpy) without the lateral packing order. While the transitions mentioned above exclusively take place within the plane of the membrane, there is the possibility of the formation of further lipid phases that make use of curvature changes involving the third dimension normal to the bilayer surface. Melting of membranes consisting of one lipid species depends on 4 factors: the length of chains, head groups, protonation and pressure.
Edge-Wiener Indices of $TUC_4C_8(R)$

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Abstract
One of topological indices which introduced very recently is edge versions of wiener index. Due to the fact that vertex version of Wiener index is very important topological index, its edge versions are important, too and they will find much applications in chemistry and mathematics such as its vertex version. In this paper, the edge-Wiener indices of $TUC_4C_8(R)$ is computed.

Keywords: Vertex-Wiener index, Edge-Wiener indices, Molecular graph, Nanotube.

References
Phase Transitions Of Membranes Consisting Of One Lipid Species

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Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran;

Abstract. A membrane represents a two-dimensional matrix embedded into three-dimensional space, which usually consists of an aqueous medium. Lipid membranes display at least two different phases: the solid-ordered phase often called the "gel phase" and the liquid-disordered phase that is often called the "fluid phase. Low temperatures lipids are arranged on a triangular lattice. At high temperatures, they do not display lateral order. Instead, they are randomly organized and represent a liquid in the language of solid state physics. For this reason the transition is called solid-liquid transition. Lipid membranes may undergo order or melting transitions. For biological membranes these transitions are typically found in the range 10-25 °C. Most lipids that are extracted from such membranes melt in the temperature regime between -20°C (some lipids with unsaturations in their chains as dioleoyl phosphatidylcholine- DOPC) and +60°C (lipids with a long saturated long chain, e.g., some sphingolipids and ceramides). Such melting transitions can be measured with many means, including differential scanning calorimetry (DSC) and various spectroscopic methods. Calorimetry has the advantage that it directly yields important thermodynamic information (e.g., enthalpy and entropy changes) not available (without interpretation) from spectroscopy.

Furthermore, the lipid chains of the individual molecules simultaneously also display order-disorder transitions. Whereas at low temperatures the lipids display predominantly all-trans configurations, at high temperatures they show a rather random chain order with many trans, gauche− and gauche+ isomerisation in their C-C
bonds in the hydrocarbon chain. These terms describe the two different ordering processes in membranes. We have found that the solid-liquid transition of the head group arrangement and the order-disorder transition of the chains do not necessarily have to occur at the same temperature and that possibly solid-disordered and liquid-ordered phases are possible. While the solid-disordered phase has so far not been identified in lipid membranes, the liquid-ordered phase has been proposed to exist in cholesterol-containing membranes, possibly due to the size of the cholesterol molecule that disturbs the formation of lateral lattices and its hydrogen bonding to carbonyl oxygen. The liquid-ordered phase is a kind of gel phase (i.e., with low enthalpy) without the lateral packing order.

While the transitions mentioned above exclusively take place within the plane of the membrane, there is the possibility of the formation of further lipid phases that make use of curvature changes involving the third dimension normal to the bilayer surface. Melting of membranes consisting of one lipid species depends on 4 factors: the length of chains, head groups, protonation, and pressure.
The Eccentric Connectivity Index of Nanostar Dendrimers

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Abstract. If $G$ is a connected graph with vertex set $V$, then the eccentric connectivity index of $G$, $\xi_c(G)$, is defined as $\sum_{v \in V} deg(v) \cdot ecc(v)$, where $deg(v)$ is the degree of a vertex $v$ and $ecc(v)$ is its eccentricity. In this paper we obtain an exact formula for calculating the eccentric connectivity index of infinite class of nanostar dendrimers.\(^1\)

Keywords: Eccentric connectivity index, Eccentricity, Nanostar dendrimer.

1. Introduction

Dendrimers are large and complex molecules with very well-defined chemical structures. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse (basically meaning of a consistent size and form) macromolecules with a regular and highly branched three-dimensional architecture. They consist of three major architectural components: core, branches and end groups. Dendrimers are produced in an iterative sequence of reaction steps. We can consider the figure of dendrimers as the shape of molecular graph.
The eccentric connectivity index, proposed by Sharma, Goswami and Madan, has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature.

Let $G$ be a simple connected graph with vertex set $V(G)$. For a vertex $v \in V(G)$, recall that $\deg(v)$ is the number of edges incident to $v$ in $G$, while $\text{ecc}(v)$ is the path length from $v$ to a vertex $u$ that is farthest from $v$, i.e., $\text{ecc}(v) = \max\{d(u, v) : u \in V(G)\}$, where $d(u, v)$ denotes the distance between $u$ and $v$ in $G$.

Sharma, Goswami and Madan introduced an adjacency-cum-distance based topological index, the eccentric connectivity index, of the graph $G$, defined as:

$$\xi^c(G) = \sum_{v \in V(G)} \deg(v) \cdot \text{ecc}(v)$$

Throughout this paper, $G[p] = \text{NSC}_2C_8h_1$ denotes the nanostar dendrimer of Figure 1. In this paper, we compute the eccentric connectivity index of nanostar dendrimers $\text{NSC}_2C_8[p]$, depicted in Figures 1 and 2.

![Fig. 1. The Nanostar Dendrimer $G[1] = \text{NSC}_2C_8[1]$](image)

2. Main Results and discussion

Here are the main results of the paper. For special classes of graphs we have the following useful results.\(^2\,3\)

**Lemma 2.1** For the complete graph $K_n$ and bipartite graph $K_{n,n}$, we have
Here, the core of generations depicted in Fig. 8. \(|V(G)| = n\) is called the order of \(G\) and the index reaches its maximum for \(K_{n,n}\) when \(a = b = n/2\).

For the star, cycle and path graphs of order \(n\),

\[
\xi^n(G) = \xi^n(K_{n+1}) = 3n^2 - 6n + 4 \quad \text{for } n \text{ even}
\]

\[
\xi^n(C_n) = \left\{ \begin{array}{ll}
\frac{n^2}{2} & \text{for } n \text{ even} \\
\frac{n(n-1)}{2} & \text{for } n \text{ odd}
\end{array} \right.
\]

\[
\xi^n(P_n) = \left\{ \begin{array}{ll}
\frac{1}{2}(3n^2 - 6n + 4) & \text{for } n \text{ even} \\
\frac{3}{2}(n-1)^2 & \text{for } n \text{ odd}
\end{array} \right.
\]

Now we compute the eccentric connectivity index of \(NSC_2C_5[b]\). Suppose \(G[n] = NSC_2C_5[b]\) denotes the molecular graph of a nanostar dendrimer with exactly \(n\) generations depicted in Fig. 1. Using an inductive argument, one can show that

\[|V(G)| = 9.2^{n+2} - 44.\]

Here, the core of \(G[n] = NSC_2C_5[b]\) has depicted in Fig. 2.

![Fig. 2. The Core of dendrimer \(G[n] = NSC_2C_5[b]\)](image)
We now partition the molecular graph of $G[n] = NSC_5C_6[6]$ into two parts, one of them is the core $C$ and other is the maximal sub graph $T$ of $G[n] = NSC_5C_6[6]$ with vertex set $V(G[n]) - V(C)$. Then we have:

**Theorem 2.2** Let $G[n] = NSC_5C_6[6]$. Then

$$\zeta^e(G[n]) = \sum_{i=1}^{n} 2^{i+1} [39(10i + 101) + 343] - 2^{n+2} (20n + 13) + 560n + 574.$$ 

**References**


THE First Geometric–Arithmetic Index Of Some Nanostar Dendrimers

A. Madanshekaf and M. Moradi

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Abstract. Dendrimers are highly branched organic macromolecules with successive layers or generations of branch units surrounding a central core [3]. These are key molecules in nanotechnology and can be put to good use. In this article, we compute the first geometric-arithmetic index of two infinite classes of dendrimers.

Keywords: nanostar dendrimer, the first geometric-arithmetic index

1. Introduction

Investigations of topological indices based on end–vertex degrees of edges have been conducted over 35 years. One of them is the first geometric–arithmetic index \( G_{A_1}(G) \). The \( G_{A_1}(G) \) index defined as:

\[
G_{A_1}(G) = \sum_{u \in V(G)} \frac{\sqrt{d_u d_v}}{2(d_u + d_v)}
\]

has been introduced less than one year ago (See Vukičević and Furtula [2]). \( d_u \) denotes degree of the vertex \( u \). Dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. The nanostar dendrimer is a part of a new group of macromolecules that appear to photon funnels just like artificial antennas. In this article many attempt have been made to compute the first geometric-arithmetic index for two types of nanostar dendrimers.
2. Results and discussions

**Lemma 1.** Consider the complete graph $K_n$ of order $n$. Then the first geometric-arithmetic index of this graph is:

$$GA_1(K_n) = \frac{1}{2}n(n-1)$$

**Lemma 2.** If $G$ is a regular graph of degree $r>0$, then

$$GA_1(G) = \frac{rn}{2}$$

**Lemma 3.** Let $S_n$ be a star on $n + 1$ vertices (Figure 1), then

$$GA_1(S_n) = \frac{2rn}{n+1}$$

For proof the reader may consult [4].

![Figure 1. Star graph with n+1 vertices](image)

2.1 The First Geometric-Arithmetic Index of the First Class of Nanostar Dendrimers

We now consider two infinite classes $NS_1[A]$ and $NS_4[A]$ of nanostar dendrimers, Figures 2 and 3. The aim of this section is to compute the first geometric-arithmetic index for two nanostar dendrimers.

We consider the molecular graph of $K(n) = NS_4[A]$ with four similar branches and three extra edges, where $n$ is steps of growth in this type of dendrimer nanostars (Figure 2).

**Theorem 4.** The first geometric-arithmetic index of $K(n) = NS_4[A]$ is computed as follows:
2.2 The Second Geometric-Arithmetic Index of the Second Class of Nanostar Dendrimers

We consider the second class \( H(n) = NS_2[D_1] \), where \( n \) is steps of growth. It is easy to see that the molecular graph of \( H \) has four similar branches and five extra edges (See Figure 3 below). Now we can state the final result.

**Theorem 5.** The first geometric-arithmetic index of \( H(n) = NS_2[D_1] \) is:

\[
G_A(H(n)) = \left( \frac{4\sqrt{3}}{3} + \frac{12\sqrt{6}}{5} \right) 2^n - \left( \frac{5 + 12\sqrt{6}}{5} \right)
\]

*Figure 2. \( NS_2[D_1] \) and \( NS_2[D_3] \) PAMAM Dendrimer*
In the following table we have provided the GA indices of these two dendrimers for \( n \geq 10 \) using Matlab Program.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \text{GA}<em>1 ) Index of ( \text{NS}</em>{1[1]} )</th>
<th>( \text{GA}<em>1 ) Index of ( \text{NS}</em>{2[1]} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>33.9525</td>
<td>20.6500</td>
</tr>
<tr>
<td>2</td>
<td>96.0862</td>
<td>52.1788</td>
</tr>
<tr>
<td>3</td>
<td>220.3537</td>
<td>115.2364</td>
</tr>
<tr>
<td>4</td>
<td>468.8886</td>
<td>241.3515</td>
</tr>
<tr>
<td>5</td>
<td>965.9583</td>
<td>493.5818</td>
</tr>
<tr>
<td>6</td>
<td>1960.1000</td>
<td>998.0424</td>
</tr>
<tr>
<td>7</td>
<td>3948.4000</td>
<td>2007.0000</td>
</tr>
<tr>
<td>8</td>
<td>7924.9000</td>
<td>4024.8000</td>
</tr>
<tr>
<td>9</td>
<td>15878.0000</td>
<td>8060.5000</td>
</tr>
<tr>
<td>10</td>
<td>31784.0000</td>
<td>16132.0000</td>
</tr>
</tbody>
</table>
Table 1. Computing GA1 index for dendrimers N2[4] and N2[4]

References


Eccentric Connectivity Index Of Some Dendrimers

K. Malekjani and M. Ghorbani

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran

Abstract. Recently a new topological index (eccentric connectivity index) was defined as $\xi(G) = \sum_{u \in V(G)} \deg_G(u)\text{ecc}(u)$, where $\deg_G(x)$ denotes the degree of the vertex $x$ in $G$ and $\text{ecc}(u) = \text{Max}\{d(x,u) | x \in V(G)\}$. In this paper we compute this topological index for some classes of dendrimers.

Keywords: Eccentric connectivity index, Dendrimers, Topological Index.
References


Topological Indices Of Non-Commuting Graph

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Abstract. Let G be a non-abelian group and let Z(G) be the center of G. Associate a graph \( \Gamma(G) \) (called noncommuting graph of G) with G as follows: Take G \( \setminus \) Z(G) as the vertices of \( \Gamma(G) \) and join two distinct vertices x and y, whenever \( xy \neq yx \). Many of theoreical properties of \( \Gamma(G) \) have been studied. In this paper we study some topological indices of non-commuting graph.

Keywords: non-commuting graph, topological index.
A Note On Eccentric Connectivity Index of Graphs

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Abstract. Let $G$ be a graph. A topological index for $G$ is a numeric quantity related to $G$ which is invariant under its automorphisms. The eccentricity of a vertex $v$ of $G$ is the maximum distance between $v$ and any other vertex of the graph. The eccentric connectivity index $\xi(G)$ of $G$ is defined as $\xi(G) = \sum_{u \in V} \text{deg}_G(u) \varepsilon(u)$ where $\text{deg}_G(u)$ denotes the degree of vertex $u$ and $\varepsilon(u)$ is the eccentricity of the vertex $u$ of the graph $G$. In this talk, we present our recent result on eccentric connectivity index of bridge and other related graphs.

Key Words: Eccentric connectivity index; bridge graph.

References

The Wiener Index of One Pentagonal Carbon Nanocone

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Abstract. Carbon nanocones form an interesting class of carbon nanomaterials which originally discovered by Ge and Sattler in 1994.1 These are constructed from a graphene sheet by removing a 60 wedge and joining the edges produces a cone with a single pentagonal defect at the apex, Figure 1. Removing additional wedges introduces more such defects and reduces the opening angle. A cone with six pentagons has an opening angle of zero and is just a nanotube with one open end.

The Wiener index of a graph G is defined as W(G) = 1/2∑_{x,y}∈V(G)d(x,y), where V(G) is the set of all vertices of G and for x,y ∈ V(G), d(x,y) denotes the length of a minimal path between x and y. In this paper we apply Klavzar’s algorithm to compute the Wiener index of one pentagonal carbon nanocone. It is proved that if H[n] = CNC_5[n] is an one-pentagonal nanocone then W(H) = (62/3)n^5 + (310/3)n^4 + (1205/6)n^3 + (1135/6)n^2 + 86n + 15.

Keywords: Nanocone, Wiener index.
Figure 1. The One Pentagonal Nanocone CNC$_3$[n].

References


On the Extremal Hexagonal Cacti for Two Types of New Indices

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Abstract. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus $G$ are cycles of the same length $m$, the cactus is $m$-uniform. A hexagonal cactus is a 6-uniform cactus, i.e., a cactus in which every block is a hexagon. Many chemical indices have been invented in theoretical chemistry. Denote $G(n, r)$ the set of cacti of order $n$ and with $r$ cycles. In this paper, we present a unified approach to the extremal cactus, which have the same or very similar structures, for two types of new indices. From our results, we can derive some known results.

References


One Type of Geometric-Arithmetic Index Of Nanotube Vphenylenic

3Sirous Moradi and Soraya Baba-Rahim*

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Abstract The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices are defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v}$, where $Q_u$ is some quantity that in a unique manner can be associated with the vertex $u$ of graph $G$. In this paper exact formulas for one type of geometric-arithmetic index of Vphenylenic nanotube are given.
On the Graph Equation $Sze(G) = We(G) + k$

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Abstract. Let $G$ be a connected graph and, $Sze(G) = We(G) + k$, where $We(G)$ and $Sze(G)$ denote the edge Wiener and edge Szeged indices of $G$, respectively. In an earlier paper, it is proved that if $T$ is a tree then $Sze(T) = We(T)$. In this paper, we continue our work to prove that for every connected graph $G$, $Sze(G) = We(G)$ if and only if $G$ is a tree. We also classify all graphs with $k < 6$. Finally, for each non-negative integer $n > 1$ there exists a graph $G$ such that $k = n$. 
Omega Polynomial in Crystal-like Networks

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b Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 400028 Cluj, Romania
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Abstract. Omega polynomial \( \Omega(G,x) \), defined by Diudea in Carpath. J. Math., 2006, 22, 43-47, counts topologically parallel edges eventually forming a strip of adjacent faces/rings, in a graph \( G=G(V,E) \). The first and second derivatives, in \( x=1 \), of Omega polynomial enables the evaluation of the Cluj-Ilmenau CI index. Analytical close formulas for the calculation of this polynomial in two hypothetical crystal-like lattices are derived.

Keywords: Omega polynomial, crystal networks.
GA₄ Index of a combined Coronene-Coronene covering

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Abstract. A new graphene pattern, called CorCor, was designed by combining the patterns of coronene [6:6₆]. The topology of the network is described in terms of geometric-arithmetic index. The geometric-arithmetic index is another topological index was defined as \( GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u) + \delta_G(v)} \), in which degree of vertex u denoted by \( \delta_G(u) \). Now we define a new version of GA index as \( GA_4(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon_G(u)\varepsilon_G(v)}}{\varepsilon_G(u) + \varepsilon_G(v)} \), in which \( \varepsilon_G(u) \) is the eccentricity of vertex u. In this paper we compute this new topological index for CorCor structure.

Keywords: Topological indices, GA Index, GA₄ Index, CorCor.
Balaban Index Of Three Classes Of Dendrimers By an Algebraic Approach

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Abstract. The Balaban index of a graph G is the first simple index of very low degeneracy. It is defined as $J(G) = m/(\mu+1) \sum e = uv[d(u)d(v)]^{-0.5}$. In this talk we report on our recent results on computing the balaban index of dendrimers using an algebraic approach. To do this we will compute the Automorphism Group of this dendrimers by wreath product formulism. Then compute the orbits of natural action of the automorphism group on dendrimers under condition.

Keywords: Balaban index, dendrimer.
Combinatorial Analysis Of RNA Structures Using Graphs

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\textbf{Abstract}. One of the important problems in Bioinformatics is the prediction of RNA structure which has received great attention during the past years. RNA structure can be expressed as a graph and so many graph theoretical problems are corresponding to the RNA structures. One of these problems deals with enumerating the number of RNA structures including some criterias (the minimum number of base pairs in stack, the minimum length for hairpin loop, etc). Our results are of importance for prediction algorithms.

\textbf{Keywords}: RNA structure, Graph, Combinatorial enumeration.
Energy Of Some Nanostructures

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Abstract. Let $G$ be a graph and $\lambda_0, \ldots, \lambda_{n-1}$, be its eigenvalues. The energy of graph is defined as $E(G) = \sum_{i=0}^{n-1} \lambda_i$. This notion is related to some applications of graph theory to chemistry and has been studied intensively in the literature, see [1,3,4,5]. In this paper we compute the energy of some nanostructures. Further, we compute energy of fullerenes $C_{20} - C_{70}$.

Keywords: Energy of graph, Nanostructures, Eigenvalue, Fullerene.

References


Computation Of the Number Of Closed Walks in Two Types Of Nano Stars

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Abstract. Let G=(V,E) be a graph. A sequence v_0v_1…v_tv_0 of vertices of a graph G is called a closed walk if v_i, v_{i+1} are in E(G), 0 \leq i \leq t – 1. In this paper, the number of closed walks of length k, CW(G, k), for two types of Nano stars are computed, where k is a positive integer.

Keywords: Nano star, closed walk.

References


Computing Nullity of Zig – Zag Nanotube

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Abstract. The nullity of a graph is defined as the multiplicity of the eigenvalue zero in the spectrum of the adjacency matrix of the graph. In this paper we compute the nullity of zig – zag nanotube, then by using this number we obtain some bounds for energy of this nanotube.

Key words: Nullity of Graphs, Nanotube, Energy of Graph.

References


The Bipartite Vertex Frustration of Some Chemical Graphs

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Abstract

Let $G=(V, E)$ be a simple graph. The Bipartite vertex frustration of $G$, denoted by $Ψ(G)$, is the smallest number of vertices that have to be deleted from a graph to obtain a bipartite subgraph. It is easy to see that $Ψ(G)$ is a topological index and $G$ is bipartite if and only if $Ψ(G)=0$. Thus $Ψ(G)$ is one of measure of bipartivity. It is well-known fact that a graph $G$ is bipartite if and only if $G$ does not have odd cycles. Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make fullerene graph bipartite. In this paper we compute the bipartite vertex frustration of some chemical graphs.

Key Words: Bipartite vertex frustration, chemical graph.

References


Extremal Catacondensed Hexagonal Systems with Respect to the GA Index

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Abstract

The concept of geometric-arithmetic index was introduced in the chemical graph theory. This index is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where $d_u$ stand for the degree of the vertex $u$. In this paper we obtain extremal catacondensed hexagonal systems with respect to the GA index.

Key words: Extremal graph, Hexagonal systems, GA index.

1. Introduction

Throughout this section $G$ is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. A topological index is a numeric quantity from the structural graph of a molecule. The concept of geometric-arithmetic index was introduced in the
chemical graph theory. This index is defined as $GA(G)=\sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v}$ where $uv$ is an edge of the molecular graph $G$ and $d_u$ stand for the degree of the vertex $u$, see [2].

A hexagonal system is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. This figure divides the plane into one infinite external region and a number of finite internal all internal region must be regular hexagons. Hexagonal systems are considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbon. A vertex of a hexagonal system belongs to at most three hexagons. A vertex shared by three hexagons is called an internal vertex; the number of internal vertices of a hexagonal system is denoted by $n_i$. A hexagonal system is called catacondensed if $n_i=0$, otherwise ($n_i>0$), it is called precondensed. In this paper we obtain extremal catacondensed hexagonal systems with respect to $GA$ index. Our notation is standard and mainly taken from [3,4].

We recall some concept about hexagonal systems that will be used in the paper. A hexagon $H$ of a catacondensed hexagonal system has either one, two or three neighboring hexagons. If $H$ has one neighboring hexagon, it is called terminal, and if it has three neighboring hexagons it is called branched. A hexagon $H$ adjacent to exactly two other hexagons posses two vertices of degree 2. If these two vertices are adjacent, $H$ is angularly connected. Each branched and angularly connected hexagons in a catacondensed hexagonal system is said to be kink, in Figure 1 the kinks are marked by K.

![Figure 1. The kinks.](image-url)
The linear chain $L_h$ with $h$ hexagons is the catacondensed system without kinks, see Figure 2. A segment is maximal linear chain in catacondensed system. The length of a segment is the number of its hexagons.

![Figure 2. A Linear Chain $L_h$.](image)

2. **Main Result and Discussion**

At first we define a concept related to a hexagonal system and use it to obtain the GA index of a hexagonal system.

**Definition 1.** A hexagon in a hexagonal system is called cubic hexagon if the degree of all vertices is equal to 3.

All of this paper, we suppose that $HS$ is a hexagonal system with $n$ vertices, $m$ edges, $h$ hexagons, $h_c$ cubic hexagons and $n_i$ internal vertices. If we partition the edge set of $HS$ into three subsets $E_1$, $E_2$ and $E_3$, as follows:

$$E_1 = \{e = uv | d_u + d_v = 4\},$$

$$E_2 = \{e = uv | d_u + d_v = 5\},$$

$$E_3 = \{e = uv | d_u + d_v = 6\}.$$ 

Therefore,
Theorem 2. Let $HS$ be a hexagonal system, then the geometric-arithmetic index is computed as follows:

$$GA_i(HS) = m + \left(\frac{2\sqrt{6}}{5} - 1\right)|E_2|.$$  \hspace{1cm} (1)

Where $k_i$ is the number of hexagons with exactly two parallel edges in $E_3$.

Corollary 3. Let $CHS$ be a catacondensed hexagonal system with $h$ hexagons. Then

$$GA_i(CHS) = \alpha h + \beta h_i - \beta k_i + 1.$$ 

Figure 3. The hexagonal system $X_{10}$

Theorem 4. Let $CHS$ be a catacondensed hexagonal system then $GA_i(L_h) \leq GA_i(CHS) \leq GA_i(X_{h'})$, (see Figure 3) and $GA_i(CHS) = GA_i(X_{h'})$ if and only if $CHS$ is a catacondensed hexagonal system with $\lfloor h \rfloor - 1$ branched and $\left\lceil \frac{h}{2} - \frac{h}{2} \right\rceil$ kinks. $GA_i(CHS) = GA_i(L_h)$ if and only if $CHS = L_h$. 

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References


A New Method for Describing Hexagonal Systems

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Abstract

A hexagonal system is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. In this paper we present a new method for describing hexagonal systems by corresponding a simple graph to each hexagonal system.

Key Words: Hexagonal System, Catacondensed.

3. INTRODUCTION

Throughout this section \(G\) is a simple connected graph with vertex and edge sets \(V(G)\) and \(E(G)\), respectively. A hexagonal system is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. This figure divides the plane into one infinite external region and a number of finite internal all internal region must be regular hexagons. Hexagonal systems
are considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbon. A vertex of a hexagonal system belongs to at most three hexagons. A vertex shared by three hexagons is called an internal vertex; the number of internal vertices of a hexagonal system is denoted by \( n_i \). A hexagonal system is called catacondensed if \( n_i = 0 \), otherwise \( n_i > 0 \), it is called precondensed. The sets of all hexagonal systems and of all hexagonal systems with \( h \) hexagons are denoted by \( HS \) and \( HS_h \), respectively. For more details about hexagonal systems, see [1, 2]. In this paper we present a new method for describing hexagonal systems by corresponding a simple graph to each hexagonal system. Our notation is standard and mainly taken from [3,4].

### 4. Main Result and Discussion

At first we define a graph related to a hexagonal system and use it to describe some hexagonal systems.

**Definition 2.1.** For each \( HS \) the related graph \( G_{HS} \) is defined as follows:

\[
V(G_{HS}) = \{H \mid H \text{ be a hexagon in hexagonal system } HS\},
\]

\[
E(G_{HS}) = \{H_1H_2 \mid \exists e \in E(X), H_1 \cap H_2 = \{e\}\}.
\]

It is easy to see that for each hexagonal system \( HS \), \( G_{HS} \) is planner and \( \Delta(G_{HS}) \leq 6 \).

**Example 2.2.** In Figure 2, there are some examples of hexagonal system and related graphs.

\[
L_5 \quad \quad \quad G_{L_5}
\]
Figure 2. Four hexagonal systems with their related graphs.
Lemma 2.2. Let $HS$ be a hexagonal system. Then the number of triangles in $G_{HS}$ is equal to the number of interval vertices.

Theorem 2.3. Let $HS$ be a hexagonal system and $G_{HS}$ its related graph. Then

$$|V(HS)| = 4|V(G_{HS})| + 2 - t(G_{HS}),$$

$$|E(HS)| = 5|V(G_{HS})| + 1 - t(G_{HS}),$$

where $t(G_{HS})$ is the number of triangles in $G_{HS}$.

Theorem 2.4. Let $G$ be a tree. If $G$ is a related graph to the hexagonal system $HS$, then $\Delta(G_{HS}) \leq 3$.

Corollary 2.5. The hexagonal system $HS$ is catacondensed if and only if $G_{HS}$ is a tree.

References


Computing GA Index of VC₅C₇[p,q], VAC₅C₇[p,q] and Nanotubes

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Abstract. In the field of chemical graph theory and in mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant-topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which biological activity or other properties of molecules are correlated with their chemical structure.

A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the wiener index, and used it to determine physical properties of types alkanes known as paraffin [2].

Topological descriptors are the numerical indices based on the topology of the atoms and their bonds. There are more than one hundred topological indices which enable us to characterize the physicochemical properties of most of molecules.

Let G be a simple connected graph, A class of Geometric-Arithmetic topological indices defined as $GA(G) = \sum_{u,v \in E(G)} 2\sqrt{Q_uQ_v} \frac{Q_u}{Q_u + Q_v}$ where $Q_u$ is some quantity associated with the vertex $u$ of G, The first class of Geometric-Arithmetic indices of G is defined as $GA(G) = $
\[ \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \text{ where } d_u \text{ is the degree of vertex } u, \text{ and the summation goes over all edges from the edge set } E(G) \] [2].

In this paper we computed the Geometric-Arithmetic index of VC\textsubscript{5}C\textsubscript{7}[p,q], VAC\textsubscript{5}C\textsubscript{7}[p,q] and VAC\textsubscript{5}C\textsubscript{6}C\textsubscript{7}[p,q] nanotubes. In fact we proved that:

\[ GA(VC\textsubscript{5}C\textsubscript{7}[p,q]) = \frac{12\sqrt{6}}{5}p + \frac{3\sqrt{3}}{2}p + 24pq - 9p. \]

\[ GA(VAC\textsubscript{5}C\textsubscript{6}C\textsubscript{7}[p,q]) = 8 \frac{\sqrt{6}}{5}pq + 24pq + 3. \]

\[ GA(VAC\textsubscript{5}C\textsubscript{7}[p,q]) = 16q \frac{\sqrt{6}}{5} + 5pq + 2q + 3. \]

**Keyword**: Topological index, Nanotubes, GA index.

**References**


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<td>Qom University</td>
</tr>
<tr>
<td>Sirwan Vaisipour</td>
<td><a href="mailto:sirwan.vaisipour@gmail.com">sirwan.vaisipour@gmail.com</a></td>
<td>Arak University</td>
</tr>
<tr>
<td>Leila Vosoughi</td>
<td>l.vosough84@gmail</td>
<td>SRTT University</td>
</tr>
<tr>
<td>Damir Vukicevic</td>
<td><a href="mailto:vukicevi@pmfst.hr">vukicevi@pmfst.hr</a></td>
<td>University of Split, Croatia</td>
</tr>
<tr>
<td>Zahra Yarahmadi</td>
<td><a href="mailto:z.yarahmadi@gmail.com">z.yarahmadi@gmail.com</a></td>
<td>Islamic Azad University of Khorram Abad</td>
</tr>
<tr>
<td>Name</td>
<td>Email</td>
<td>Institution</td>
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<tr>
<td>Lida Zabolizadeh</td>
<td><a href="mailto:l_zaboli@yahoo.com">l_zaboli@yahoo.com</a></td>
<td>Yazd University</td>
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<tr>
<td>Malihe Zeraatkar</td>
<td><a href="mailto:m.zeraatkar@modares.ac.ir">m.zeraatkar@modares.ac.ir</a></td>
<td>Tarbiat Modares University</td>
</tr>
<tr>
<td>Bo Zhou</td>
<td><a href="mailto:zhoubo@scnu.edu.cn">zhoubo@scnu.edu.cn</a></td>
<td>South China Normal University, China</td>
</tr>
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# Wednesday

<table>
<thead>
<tr>
<th>Time</th>
<th>Name &amp; Family</th>
<th>Chairman</th>
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</thead>
<tbody>
<tr>
<td>9:00–10:00</td>
<td>Haruo Hosoya</td>
<td>Tomislav Doslic</td>
</tr>
<tr>
<td>10:00 – 10:30</td>
<td>Ardeshir Dolati</td>
<td>Tomislav Doslic</td>
</tr>
<tr>
<td>10:30 – 11:00</td>
<td><strong>COFFEE BREAK</strong></td>
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</tr>
<tr>
<td>11:00 – 12:00</td>
<td>Ante Graovac</td>
<td>Damir Vukicevic</td>
</tr>
<tr>
<td>12:00 – 12:15</td>
<td>Roghieh Hafezieh</td>
<td>Damir Vukicevic</td>
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<tr>
<td>12:15 – 12:30</td>
<td>Afshin Behmaram</td>
<td>Damir Vukicevic</td>
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<tr>
<td>12:30 – 12:45</td>
<td>Khadijeh Fathalikhani</td>
<td>AliReza Ashrafi</td>
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<tr>
<td>12:45 – 13:00</td>
<td>Zohreh Mohammad Abadi</td>
<td>AliReza Ashrafi</td>
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<tr>
<td>13:00 – 15:00</td>
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<tr>
<td>15:30 – 16:30</td>
<td>Tomislav Doslic</td>
<td>Bo Zhou</td>
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<tr>
<td>16:30 – 16:45</td>
<td>Mohammad A. Iranmanesh</td>
<td>Bo Zhou</td>
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<tr>
<td>16:45 – 17:00</td>
<td>Mahsa Mirzargar</td>
<td>Bo Zhou</td>
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<td>17:30 – 18:30</td>
<td><strong>POSTER Session</strong></td>
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# Thursday

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<tr>
<td>8:20 – 9:20</td>
<td>Damir Vukicevic</td>
<td>Saeid Akbari</td>
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<tr>
<td>9:20 – 9:35</td>
<td>Saeid Alikhani</td>
<td>Saeid Akbari</td>
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<tr>
<td>9:35 – 9:50</td>
<td>Zahra Yarahmadi</td>
<td>Saeid Akbari</td>
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<tr>
<td>9:50 – 10:05</td>
<td>Mojgan Mogharrab</td>
<td>Saeid Akbari</td>
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<td>10:05 – 10:20</td>
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<td>10:20 – 11:20</td>
<td>Bo Zhou</td>
<td>Ante Graovac</td>
</tr>
<tr>
<td>11:20 – 11:35</td>
<td>Azizollah Azad</td>
<td>Ante Graovac</td>
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<td>11:35 – 11:50</td>
<td>Sirous Moradi</td>
<td>Ante Graovac</td>
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<tr>
<td>11:50 – 12:05</td>
<td>Mohammad J. Nadjafi</td>
<td>Haruo Hosoya</td>
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<tr>
<td>12:05 – 12:20</td>
<td>Mandana Ghaneei</td>
<td>Haruo Hosoya</td>
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<td>12:20 – 14:30</td>
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<tr>
<td>14:30 – 14:45</td>
<td>Mahsa Ghazi</td>
<td>Mohammad A. Iranmanesh</td>
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<tr>
<td>14:45 – 15:00</td>
<td>Hossein Shabani</td>
<td>Mohammad A. Iranmanesh</td>
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<td>15:00 – 15:30</td>
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