

Geometric–arithmetic Indices

Boris Furtula and Ivan Gutman

*Faculty of Science, University of Kragujevac, P. O. Box 60,
34000 Kragujevac, Serbia*
furtula@kg.ac.rs & gutman@kg.ac.rs

The concept of geometric–arithmetic indices (GA) was introduced in the chemical graph theory very recently. In spite of this, several papers have already appeared dealing with these indices. The main goal of this survey is to collect all hitherto obtained results on GA indices (both chemical and mathematical).

1. Introduction

Molecular descriptors play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. Among them, special place is reserved for so-called topological descriptors. Nowadays, there exists a legion of topological indices that found some applications in chemistry [1]. They can be classified by the structural properties of graphs used for their calculation. Hence, probably the best known and widely used Wiener index [2] is based on topological distance of vertices in the respective graph, the Hosoya index [7] is calculated counting of non-incident edges in a graph, the energy [3] and the Estrada index [4] are based on the spectrum of the graph, the Randić connectivity index [5] and the Zagreb group indices [6] are calculated using the degrees of vertices, etc.

Here, a new class of topological descriptors, based on some properties of vertices of graph is presented. These indices are named as “*geometric–arithmetic indices*” ($GA_{general}$) and their definition is as follows [9]:

$$GA_{general} = GA_{general}(G) = \sum_{uv \in E(G)} \frac{\sqrt{Q_u Q_v}}{\frac{1}{2}(Q_u + Q_v)} \quad (1)$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G .

The name of this class of indices is evident from their definition. Namely, indices belonging to this group are calculated as the ratio of geometric and arithmetic means of some properties of adjacent vertices u and v (vertices u and v are connected by an edge). Summation goes over all edges in a respective graph G . Three members of GA group topological indices are put forward up to now.

The first member [8] is the so-called *geometric–arithmetic index* GA_1 , defined as

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

where uv is an edge of the (molecular) graph G connecting the vertices u and v , where d_u stands for the degree of the vertex u , and where the summation goes over all edges of G .

In the rest of the text we are calling it as the “*first geometric–arithmetic index*”.

Another member of this class we denote by GA_2 and is – tentatively – referred to as the *second geometric–arithmetic index*. Whereas GA_1 is defined so as to be related to the famous Randić index [5], GA_2 is constructed in such a manner that it is related with Szeged [10] and vertex Padmakar–Ivan [11] indices (see below).

Let G be a connected graph with n vertices and m edges, with vertex set $V(G)$ and edge set $E(G)$. As usual [12], the distance $d(x, y|G)$ between two vertices $x, y \in V(G)$ is defined as the length (= number of edges) of the shortest path that connects x and y . Let $e = uv$ be an edge of G , connecting the vertices u and v . Define the sets

$$\mathbf{N}(e, u, G) = \{x \in V(G) \mid d(x, u|G) < d(x, v|G)\}$$

$$\mathbf{N}(e, v, G) = \{x \in V(G) \mid d(x, u|G) > d(x, v|G)\}.$$

consisting, respectively, of vertices of G lying closer to u than to v , and lying closer to v than to u . The number of such vertices is then

$$n_u(e) = n_u(e, G) = |\mathbf{N}(e, u, G)| \quad \text{and} \quad n_v(e) = n_v(e, G) = |\mathbf{N}(e, v, G)|. \quad (3)$$

Note that vertices equidistant to u and v are not included into either $\mathbf{N}(e, u, G)$ or $\mathbf{N}(e, v, G)$. Such vertices exist only if the edge uv belongs to an odd-membered cycle. Hence, in the case of bipartite graphs, $\mathbf{N}(e, u, G) \cup \mathbf{N}(e, v, G) = V(G)$ and, consequently,

$$n_u(e, G) + n_v(e, G) = n \quad (4)$$

for all edges of the graph G .

It is also worth noting that $u \in \mathbf{N}(e, u, G)$ and $v \in \mathbf{N}(e, v, G)$, which implies that $n_u(e) \geq 1$ and $n_v(e) \geq 1$.

Motivated by the expressions for calculation of Szeged (Sz) and recently introduced vertex Padmakar–Ivan (PI_v) indices, and in view of the general formula (1), the *second geometric–arithmetic index* is defined as

$$GA_2 = GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u \cdot n_v}}{\frac{1}{2}[n_u + n_v]}. \quad (5)$$

Currently, the last introduced topological index belonging to the GA class is the so-called the “*third geometric–arithmetic index*”, denoted as GA_3 [13]. In order to define the GA_3 index, some preparation must be done.

Let x be a vertex and uv be an edge of the graph G . The distance between x and uv is defined as $d(x, uv|G) = \min\{d(x, u|G), d(x, v|G)\}$. For $uv \in E(G)$, let $m_u = |\{f \in E(G) : d(u, f|G) < d(v, f|G)\}|$.

It should be noted that m_u is not a quantity that in a unique manner can be associated with the vertex u of the graph G , but that it depends on the edge uv . Yet, this restriction is not relevant for the definition of GA_3 . Note that in all cases $m_u \geq 0$ and $m_u + m_v \leq m - 1$.

Then, incorporating m_u as vertex quantity into Eq. (1) the *third geometric–arithmetic index* is defined as

$$GA_3 = GA_3(G) = \sum_{uv \in E(G)} \frac{\sqrt{m_u \cdot m_v}}{\frac{1}{2}[m_u + m_v]}. \quad (6)$$

Similarly to GA_2 , the *third geometric–arithmetic index* is defined as to be related to the recently introduced edge Szeged (Sz_e) index [14] and edge Padmakar–Ivan (PI_e) index [15].

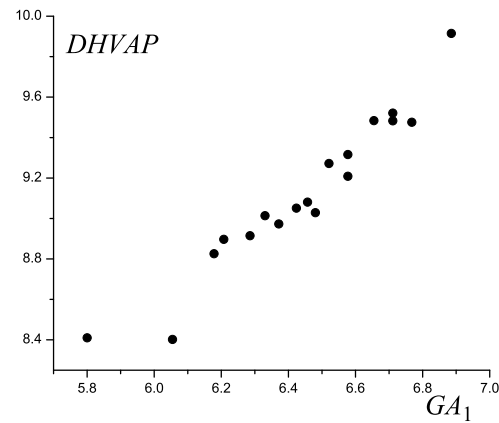
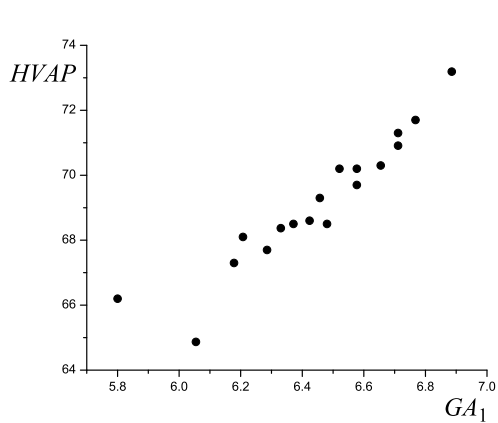
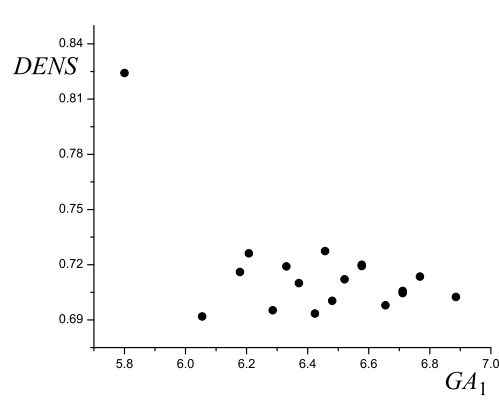
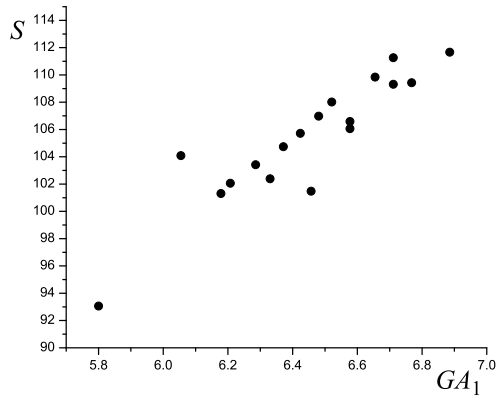
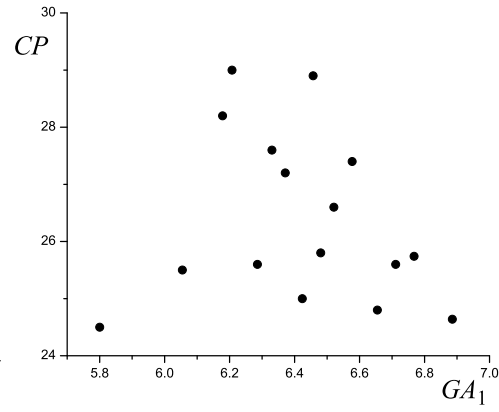
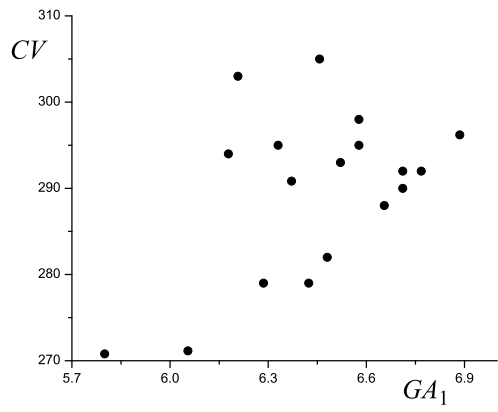
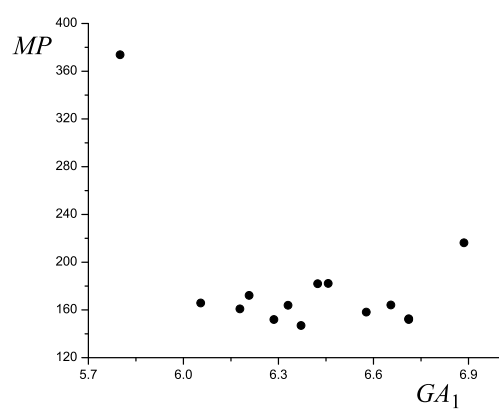
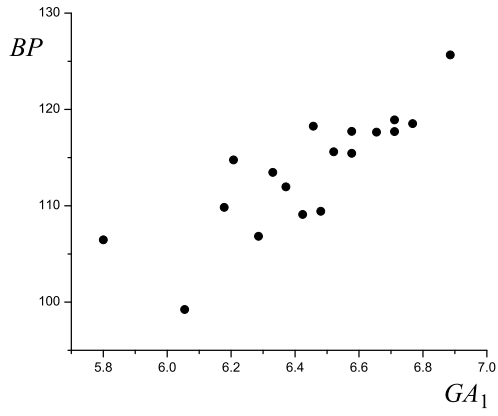
2. The First Geometric–arithmetic Index

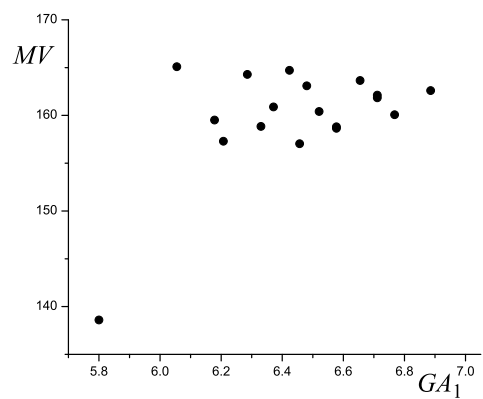
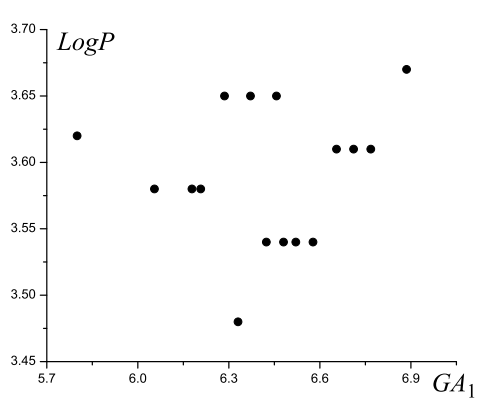
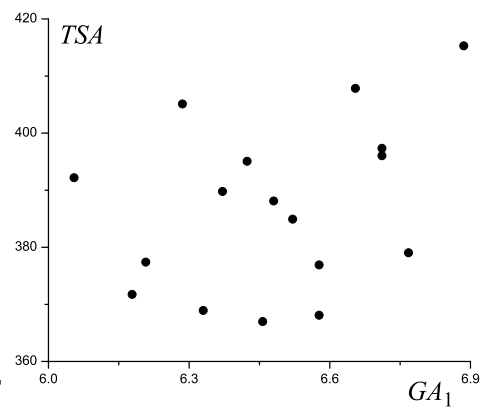
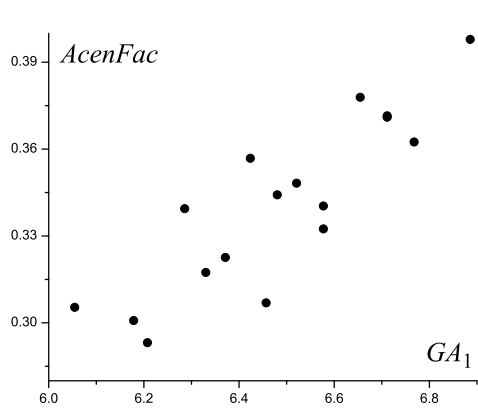
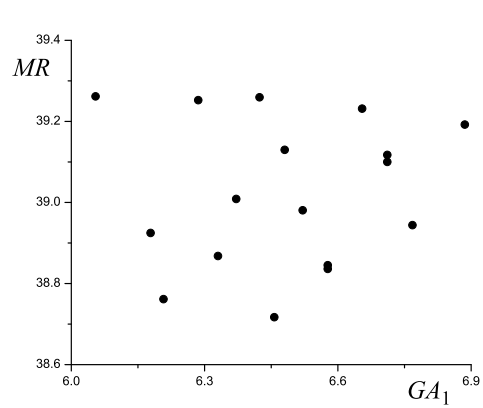
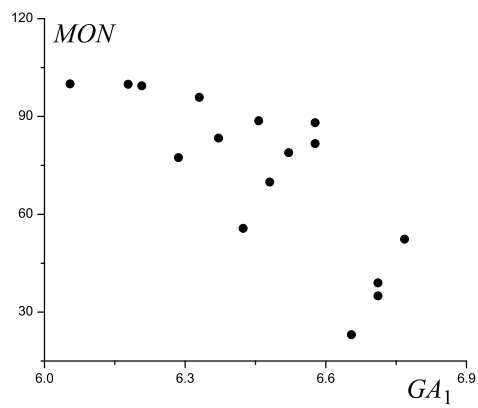
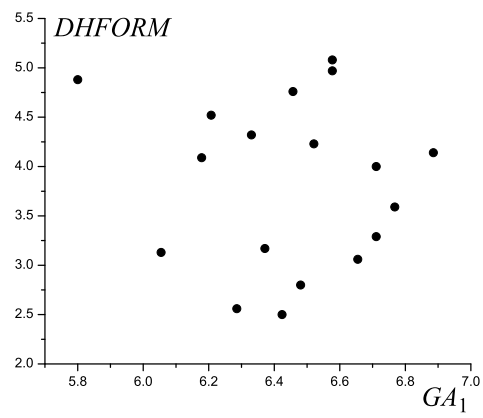
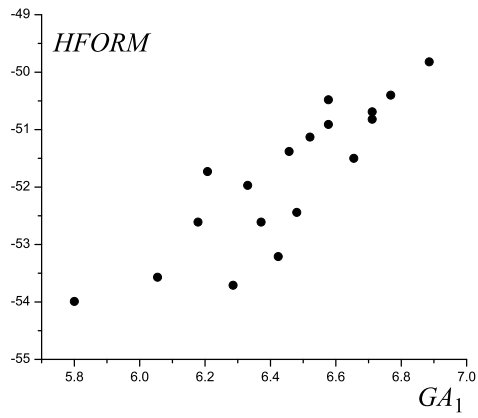
Investigations of topological indices based on end–vertex degrees of edges have been conducted over 35 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index (χ) [5]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (for example see [16–18] and the references cited therein). During years of research, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a number of modifications and new topological descriptors resembling the original χ –index. The *first geometric–arithmetic index* (GA_1) may be viewed as one of the successors of the Randić connectivity index.

The GA_1 index, defined by Eq. (2), has been introduced less than a year ago [8]. However, a few papers are appeared dealing with this quantity. In the subsequent section, the results on GA_1 will be summarized.

2.1. GA_1 as a tool for QSAR/QSPR researches

The reason for introducing a new index is to gain prediction of target property (properties) of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new index must be done. As a “standard” for testing new topological descriptors, the properties of octanes are commonly used. A benchmark data sets can be found at www.moleculardescriptors.eu. This data set contains 16 physico–chemical properties of octanes: boiling point (BP), melting point (MP), heat capacity at V constant (CV), heat capacity at P constant (CP), Entropy (S), density ($DENS$), enthalpy of vaporization ($HVAP$), standard enthalpy of vaporization ($DHVAP$), enthalpy of formation ($HFORM$), standard enthalpy of formation ($DHFORM$), motor octane number (MON), molar refraction (MR), acentric factor ($AcenFac$), total surface area (TSA), octanol–water partition coefficient ($LogP$), and molar volume (MV). The correlations between the GA_1 index and these physico–chemical properties are given on the following figures:





In [8], the predictive ability of GA_1 was compared with that of the Randić connectivity index using the following physico-chemical properties of octanes: Boiling point (BP), Entropy (S), Enthalpy of vaporization ($HVAP$), Standard enthalpy of vaporization ($DHVAP$), Enthalpy of formation ($HFORM$), and Acentric factor ($AcenFac$). The motivation for choosing just these physico-chemical properties is that both GA_1 and the Randić connectivity indices give relatively good linear correlations, i. e., the respective correlation coefficients are greater than 0.8. The results are presented in Table 1.

	Correlation coefficient (R)		$1 - RQR(\%)$
	GA_1 index	Randić index	
BP	0.823	0.821	0.562
S	0.912	0.906	2.942
$HVAP$	0.941	0.936	4.152
$DHVAP$	0.966	0.958	9.005
$HFORM$	0.858	0.850	2.494
$AcenFac$	0.912	0.904	4.051

Table 1. Correlation coefficients for GA_1 and Randić index and some physico-chemical properties of octanes. RQR is the ratio of quadratic mean of residuals.

A superficial glance on R 's does not justify the introduction of the GA_1 index because (even though the GA_1 gives better correlation coefficients than χ) the differences between them are not significant. However, the predicting ability of the GA_1 index compared with Randić index is reasonably better, which is indicated by the ratio of quadratic mean of residuals, RQR ¹(see Table 1).

Benzenoid hydrocarbons (B) belong to the most important polycyclic aromatic compounds. They consist of fused benzene rings. Their characteristic physico-chemical properties, especially their thermal stability, was subject to intensive research. Benzenoid hydrocarbons found a number of applications in industry. They are also big pollutants and some of them are carcinogenic chemicals. Nowadays, there are numerous published researches, both experimental and theoretical, dealing with this class of molecules. More information about them can be found in the book [24] and the references cited therein.

¹The RQR value can be calculated using the following formula

$$RQR = \sqrt{\frac{\sum_{i=1}^n [a(GA_1)_i + b - Exp_i]^2}{\sum_{i=1}^n [a'\chi_i + b' - Exp_i]^2}}$$

Whereas nowadays only ca. 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is unimaginatively large. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5851000265625801806530 [25]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species.

Here, the heat of formation of 25 benzenoid hydrocarbons is modeled using the GA_1 index. The data set, collected from the article [26], is given in Table 2.

Name	n	ΔH_f (g) (kJ/mol)	GA_1
benzene	6	82.9	6.000
naphthalene	10	150.6	10.919
anthracene	14	227.7	15.838
phenanthrene	14	207.1	15.879
pyrene	16	225.7	18.838
benzo[<i>a</i>]anthracene	18	291.0	20.798
benzo[<i>c</i>]phenanthrene	18	302.4	20.838
chrysene	18	262.8	20.838
naphacene	18	291.4	20.758
triphenylene	18	269.8	20.879
benzo[<i>a</i>]pyrene	20	301.0	23.798
benzo[<i>e</i>]pyrene	20	304.0	23.838
perylene	20	324.0	23.838
benzo[<i>b</i>]chrysene	22	346.0	25.758
benzo[<i>c</i>]chrysene	22	334.0	25.798
benzo[<i>g</i>]chrysene	22	333.0	25.838
benzo[<i>a</i>]naphacene	22	359.0	25.717
dibenzo[<i>a,c</i>]anthracene	22	345.0	25.798
dibenzo[<i>a,h</i>]anthracene	22	343.0	25.758
dibenzo[<i>a,j</i>]anthracene	22	343.0	25.758
dibenzo[<i>b,g</i>]phenanthrene	22	347.0	25.758
dibenzo[<i>c,g</i>]phenanthrene	22	335.0	25.798
pentacene	22	374.5	25.677
pentaphene	22	359.0	25.717
picene	22	334.0	25.798

Table 2. Heat of formation and the GA_1 index of some benzenoid hydrocarbons

The correlation graphic between the GA_1 indices and heat of formation of the 25 benzenoid hydrocarbons from Table 2 is shown in Fig. 1. It is evident from this graphic that between GA_1 and the heat of formation of benzenoid hydrocarbons there exists a good linear correlation. The respective correlation coefficient is equal to 0.972.

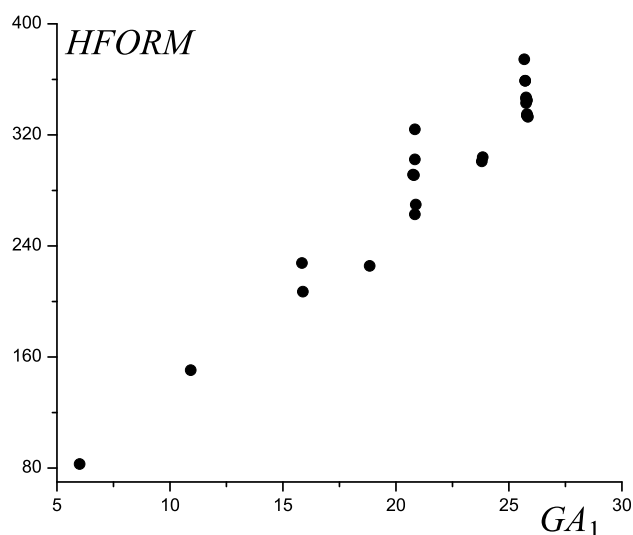


Figure 1. Heat of formation vs. GA_1 for the 25 benzenoid hydrocarbons from Table 2.

However, it is well known that the heat of formation roughly depends on the number of atoms in the molecule, and therefore the correlation shown in Fig. 1 may, in fact, look unrealistically good. In order to overcome this problem, the examination of correlation between heat of formation and GA_1 index should be limited to isomers. Among experimental results given in Table 1 there are all twelve catacondensed² benzenoid hydrocarbons with 5 benzene rings (i. e., 22 carbon atoms). The correlation between the GA_1 index and heat of formation for the 12 catacondensed benzenoid hydrocarbons with 5 benzene rings is shown in Fig. 2.

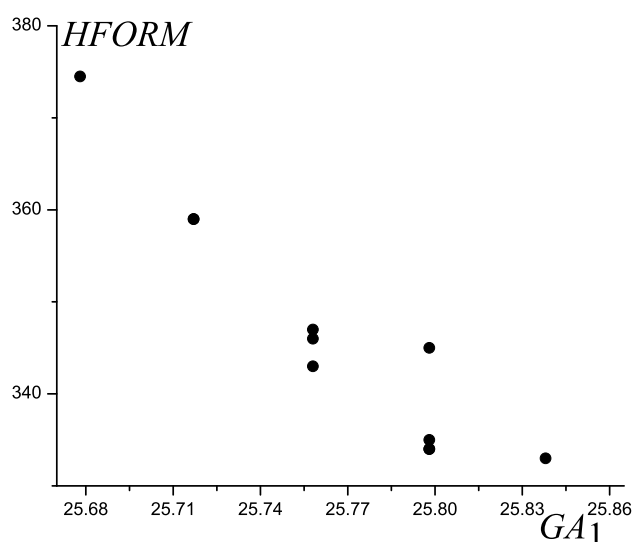


Figure 2. Correlation between GA_1 and the heat of formation for all catacondensed benzenoid hydrocarbons with 5 hexagons (i. e., with 22 carbon atoms)

²Benzenoid hydrocarbons containing no internal carbon atoms (carbon atoms belonging to three six-membered rings) are said to be “catacondensed”.

The correlation coefficient is -0.939 . It should be noted from Fig. 2 that two outliers exist. By inspecting the data set of twelve catacondensed benzenoid hydrocarbons with 5 benzene rings, we determined which molecules correspond to these two outliers. These are benzo[*g*]chrysene and dibenz[*a,c*]anthracene, the only two branched catacondensed benzenoid hydrocarbons in this data set. This observation leads to the conclusion that for the modeling of the heat of formation of benzenoid hydrocarbons, other structural details should be incorporated beside the GA_1 index.

2.2. Mathematical properties of the GA_1 index

In this subsection, the mathematical results on the *first geometric–arithmetic index* are presented. All results apply to simple graphs, i. e., to graphs without loops, multiple edges, and directed edges.

2.2.1. Lower and upper bounds for GA_1

Knowing the fact that the geometric mean is less than or equal to the arithmetic mean, it is obvious that all indices belonging to the GA class satisfy $GA_{general} \leq m$. In addition, it is evident from Eq. (1) that $GA_{general}$ is equal to 0 for an empty graph. Taking that into account we get for all simple graphs

$$0 \leq GA_{general}(G) \leq m \leq \binom{n}{2}. \quad (7)$$

The equality on the righthand side of (7) is attained if and only if G is a regular graph with $\binom{n}{2}$ edges. The only such graph is the complete graph (K_n).

Eq. (7) applied to GA_1 yields the first inequality for that index [8]:

$$0 = GA_1(\overline{K}_n) \leq GA_1(G) \leq \binom{n}{2} = GA_1(K_n)$$

where \overline{K}_n is the complement graph of the complete graph K_n . In other words, this is the empty graph with n vertices.

In [8], the following inequality is obtained for all connected simple graphs with n vertices:

$$\frac{2(n-1)^{3/2}}{n} = GA_1(S_n) \leq GA_1(G) \leq \binom{n}{2} = GA_1(K_n).$$

The lower bound is achieved if and only if G is the star (S_n) and the upper bound is the same as for all graphs.

The authors of [19] found for triangle-free graphs with n vertices and m edges the inequality

$$GA_1(G) \geq \left(\frac{2m}{n}\right)^2,$$

with equality attained if and only if G is the regular complete bipartite graph.

In the paper [20], a lower bound for GA_1 of a simple graph G with m edges, in terms of maximum vertex degree (Δ) and minimum vertex degree (δ) was presented.

$$GA_1(G) \geq \frac{2m\sqrt{\Delta \cdot \delta}}{\Delta + \delta}.$$

Equality holds if and only if G is a regular graph or G is a bipartite semi-regular graph.

Also, in [20] a lower and an upper bound for GA_1 was reported in following terms:

δ_1 – minimum non-pendent vertex degree

d_1, d_2, \dots, d_n – degree sequence

$M_2(G)$ – second Zagreb index

p – number of pendent vertices

$m - p = \mu$ – number of non-pendent edges

$$\frac{2p\sqrt{\Delta}}{\Delta + 1} + \sqrt{\mu^2 - \frac{\mu}{4\delta_1^2} \left[\sum_{i=1}^n d_i^3 - 2M_2(G) - p(\delta_1 - 1)^2 \right] - \frac{\mu^2}{4} \left(1 - \frac{2\sqrt{\Delta\delta_1}}{\Delta + \delta_1} \right)^2}$$

$$\leq GA_1(G) \leq$$

$$\frac{2p\sqrt{\delta_1}}{\delta_1 + 1} + \sqrt{\mu^2 - \frac{\mu}{4\Delta^2} \left[\sum_{i=1}^n d_i^3 - 2M_2(G) - p(\Delta - 1)^2 \right]}.$$

The lower and upper bounds are equal when G is a regular graph or a $(\Delta, 1)$ -semiregular graph.

Nordhaus–Gaddum type [21] lower and upper bounds for a connected graph G and its connected complement graph \overline{G} were obtained in [20]:

$$\frac{2k}{k^2 + 1} \binom{n}{2} \leq GA_1(G) + GA_1(\overline{G}) \leq \binom{n}{2} - p \frac{(\sqrt{\delta_1} - 1)^2}{\delta_1 + 1} - \overline{p} \frac{(\sqrt{\overline{\delta_1}} - 1)^2}{\overline{\delta_1} + 1}$$

where $k = \max \left\{ \sqrt{\frac{\Delta}{\delta}}, \sqrt{\frac{n-1-\delta}{n-1-\Delta}} \right\}$. p , \overline{p} , and δ_1 , $\overline{\delta_1}$ are the number of pendent vertices and minimum non-pendent vertex degrees in G and \overline{G} , respectively.

The lower and upper bounds are equal when G is a regular graph.

2.2.1.1. Lower and upper bounds for GA_1 of molecular graphs

A connected graph with maximum vertex degree at most 4 is said to be a “*molecular graph*”. Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in chemistry. Nowadays this area of mathematical chemistry is called *chemical graph theory* [22].

In [19], lower and upper bounds for molecular graph G with $n \geq 4$ vertices and $m \in [n - 1, 2n]$ edges are given:

$$\frac{17m - 4n}{15} \leq GA_1(G) \leq \frac{1}{3} \left[(9 - 4\sqrt{2})m - (6 - 4\sqrt{2})n \right].$$

The left equality is attained if and only if G has only the vertices of degree four and one. The right equality is reached if and only if the G is a path or a cycle.

2.2.2. Lower and upper bounds for GA_1 of trees

The simplest connected graphs are the trees (T). Hence, the mathematical properties of some graph invariant are usually first investigated on them.

Therefore, the authors of the paper [8] explored mathematical properties of GA_1 of trees and chemical trees. They obtained the following tight lower and upper bounds for trees:

$$\frac{2(n-1)^{3/2}}{n} = GA_1(S_n) \leq GA_1(T) \leq GA_1(P_n) = \begin{cases} 0 & n = 1 \\ 1 & n = 2 \\ \frac{4\sqrt{2}}{3} + n - 3 & n \geq 3 \end{cases} \quad (8)$$

The lower bound is achieved if and only if T is the star (S_n), and the upper bound is achieved if and only if T is the path (P_n).

2.2.2.1. The GA_1 index of chemical trees

A tree in which the maximum vertex degree does not exceed 4 is said to be a “*chemical tree*”. Since a path is a chemical tree, the upper bound for chemical trees is the same as in the inequality (8). The lower bound for chemical trees is given in [8]:

$$GA_1(T) \geq \frac{13n - 17}{15} .$$

The equality holds for chemical trees containing only vertices of degrees one and four. In other words, the chemical tree(s) with $n = 3k + 2$, $k = 1, 2, \dots$, vertices are those with minimal GA_1 index.

Among chemical trees with $n = 3k + 2$ vertices the minimal GA_1 index may belong to more than one tree. In Table 3 are given the numbers of chemical trees having minimal GA_1 index up to 20 vertices.

n	η
5	1
8	1
11	1
14	2
17	3
20	5

Table 3 Among chemical trees with n vertices there are η trees having minimal GA_1 index.

In the paper [19] chemical trees with first, second, and third minimal GA_1 index were determined. Three cases can be distinguished:

Case I: If $n \equiv 2 \pmod{3}$, then among the n -vertex chemical trees,

- (a) for $n \geq 5$, the ones with only degrees 1 and 4 are the trees with minimum GA_1 index, which is equal to $\frac{13n-17}{15}$;
- (b) for $n \geq 17$, the ones with a single vertex of degree 2 adjacent to two vertices of degree 4, and a single vertex of degree 3 adjacent to three vertices of degree 4 are the chemical trees having second minimum GA_1 index equal to $\frac{13}{15}n + \frac{12\sqrt{3}}{7} + \frac{4\sqrt{2}}{3} - \frac{89}{15}$;
- (c) for $n \geq 17$, the ones with three vertices of degree 2, each adjacent to two vertices of degree 4, and without vertices of degree 3 are the chemical trees with third minimum GA_1 index equal to $\frac{13n+60\sqrt{2}-101}{15}$.

Case II: If $n \equiv 1 \pmod{3}$, then among the n -vertex chemical trees,

- (a) for $n \geq 13$, the ones with a single vertex of degree 3 adjacent to three vertices of degree 4, and without vertices of degree 2 are the chemical trees with the minimum GA_1 index equal to $\frac{13}{15}n + \frac{12\sqrt{3}}{7} - \frac{61}{15}$;
- (b) for $n \geq 13$, the ones with two vertices of degree 2 adjacent to four vertices of degree 4, and without vertices of degree 3 are the chemical trees with the second minimum GA_1 index equal to $\frac{13n+40\sqrt{2}-3}{15}$;
- (c) for $n \geq 25$, the ones with a single vertex of degree 2 adjacent to two vertices of degree 4, and two vertices of degree 3, each adjacent to three vertices of degree 4 are the chemical trees with the third minimum GA_1 index equal to $\frac{13}{15}n + \frac{4\sqrt{2}}{3} + \frac{24\sqrt{3}}{7} - \frac{133}{15}$.

Case III: If $n \equiv 0 \pmod{3}$, then among the n -vertex chemical trees,

- (a) for $n \geq 9$, the ones with a single vertex of degree 2 adjacent to two vertices of degree 4, and without vertices of degree 3 are the chemical trees with minimum GA_1 index equal to $\frac{13n+20\sqrt{2}-45}{15}$;
- (b) for $n \geq 21$, the ones with two vertices of degree 3, each adjacent to three vertices of degree 4, and without vertices of degree 2 are the chemical trees with second minimum GA_1 index equal to $\frac{13}{15}n + \frac{24\sqrt{3}}{7} - 7$;
- (c) for $n \geq 21$, the ones with two vertices of degree 2, each adjacent to two vertices of degree 4, and a single vertex of degree 3 adjacent to three vertices of degree 4 are the chemical trees with the third minimum GA_1 index equal to $\frac{13}{15}n + \frac{8\sqrt{2}}{3} + \frac{12\sqrt{3}}{7} - \frac{39}{5}$.

In addition, the same authors determined the chemical trees with second and third maximal GA_1 index.

- (a) Among all n -vertex chemical trees, the path is the unique tree with the maximum GA_1 index equal to $n - 3 + \frac{4\sqrt{2}}{3}$;
- (b) for $n \geq 7$ the chemical trees possessing a single vertex of degree 3 adjacent to three vertices of degree 2 and without vertices of degree 4 are the trees with second maximum GA_1 index equal to $n - 7 + 2\sqrt{2} + \frac{6\sqrt{6}}{5}$;

(c) for $n \geq 7$ the ones with a single vertex of degree 3 adjacent to two vertices of degree 2 and one vertex of degree 1, and without vertices of degree 4 are the chemical trees with third maximum GA_1 index equal to $n - 6 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$.

2.2.3. GA_1 index of benzenoid hydrocarbons and phenylenes

Benzenoid systems (graph representations of benzenoid hydrocarbons) are defined as finite plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. One example of benzenoid hydrocarbon is given in Fig. 3 (a). Hexahelicene (Fig. 3 (b)) does not belong to the class of benzenoid hydrocarbons because it does not obey the condition of planarity.

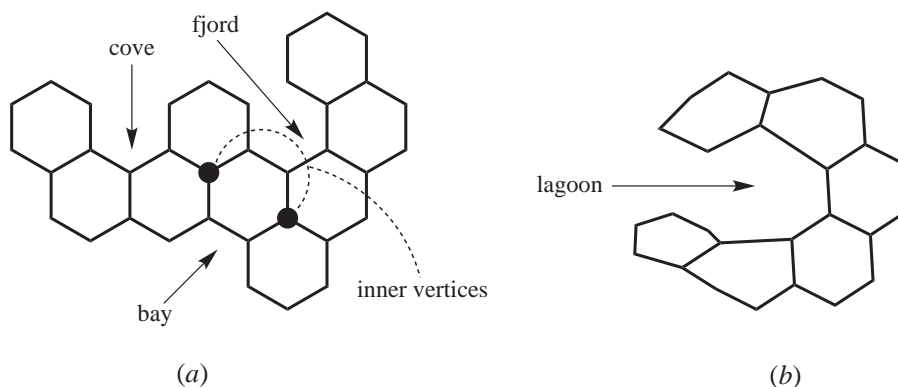


Figure 3. (a) dinaphtho[1,2- a :2',1'- k]perylene possesses all structural properties that can be found on the perimeter of a benzenoid system; (b) ordinary benzenoid hydrocarbons do not possess structural details called lagoon. Phenanthro[3,4- c]phenanthrene (hexahelicene) is the first member of a class of molecules referred to as helicenes and it has a lagoon.

Phenylenes are a class of alternant polycyclic conjugated molecules consisting of six- and four-membered rings, so that each four-membered ring is adjacent to two (disjoint) six-membered rings, and no two six-membered rings are adjacent. K. P. C. Vollhardt with his group synthesized a large number of phenylenes (for details see [27,28]). They attracted much attention of theoretical chemists because of their specific structure (containing both stabilizing six-membered, and destabilizing four-membered rings) [29–31]. Structural features such as bays, coves, fjords, and lagoons can be found also in the structural formulas of phenylenes (see Fig. 4(a)). The phenylenes do not have inner vertices. Numerous theoretical researches had shown that there exist relations between a number of topological descriptors of a phenylene and its hexagonal squeeze, HS , (benzenoid hydrocarbon which topology corresponding to the considered phenylene) [31–42].

In other words, each phenylene is in a one-to-one correspondence with a catacondensed benzenoid hydrocarbon called hexagonal squeeze. The construction of the hexagonal squeezes of phenylenes should be obvious from Fig. 4(b).

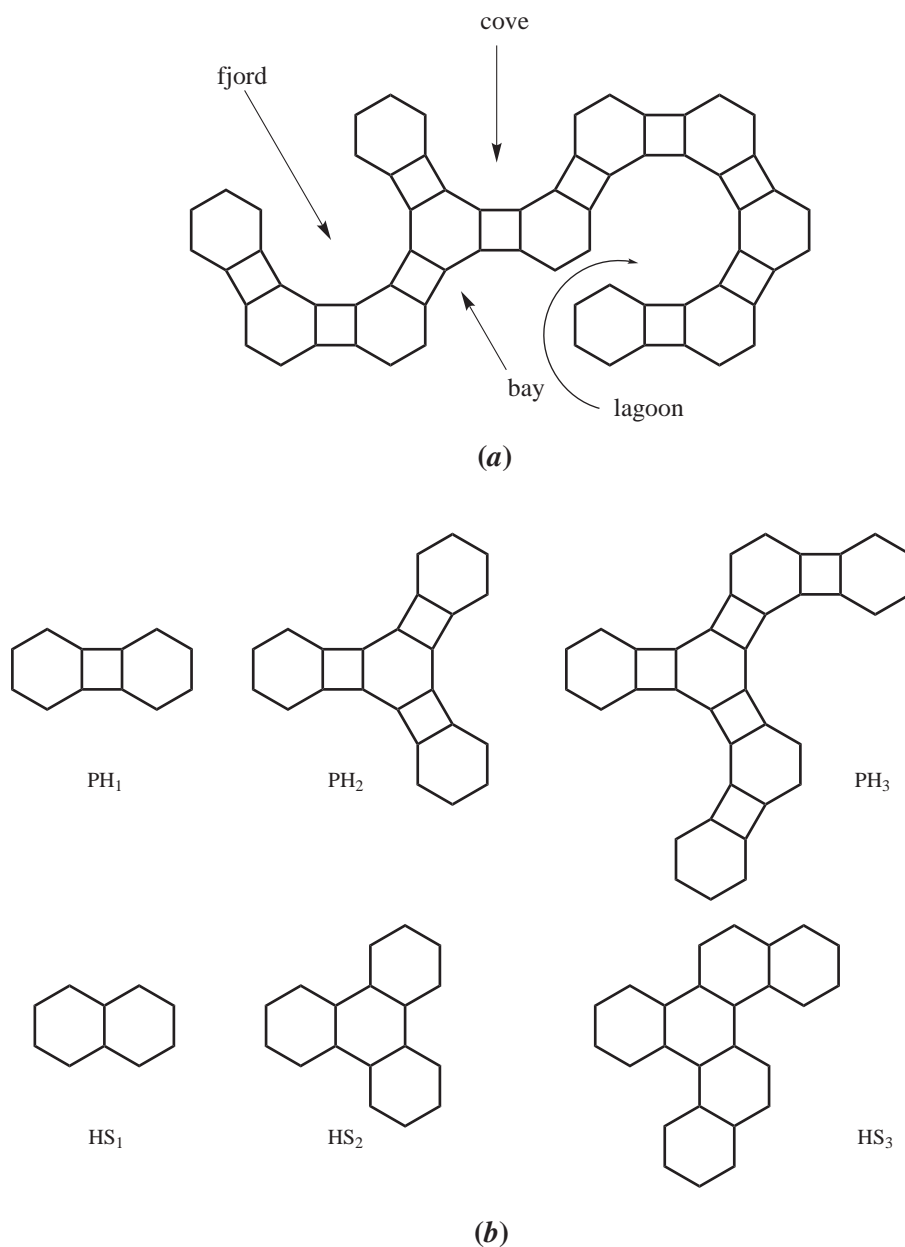


Figure 4. (a) Phenylenes possess all structural properties noticed already in benzenoid hydrocarbons (cf. Fig. 3), except inner vertices. (b) Phenylenes PH_1 , PH_2 , PH_3 and the corresponding hexagonal squeezes HS_1 , HS_2 , HS_3 .

Names of structural features that are used here and notations of their counts is in accordance with the terminology proposed by Cyvin and one of the present authors [23, 24]. Thus,

n_i	=	number of inner vertices
h	=	number of hexagons
B	=	number of bays
C	=	number of coves
F	=	number of fjords
L	=	number of lagoons
b	=	number of bay regions; $b = B + 2C + 3F + 4L$

Using the above specified structural parameters, it is easy to derive the exact formula for calculation of the GA_1 index of benzenoid hydrocarbons:

$$GA_1(B) = \frac{8\sqrt{6} + 5}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{4\sqrt{6} - 5}{5}n_i - \frac{8\sqrt{6} - 25}{5}. \quad (9)$$

For catacondensed benzenoid hydrocarbons (i. e., hexagonal squeezes) Eq. (9) is reduced by deleting the term $\frac{4\sqrt{6}-5}{5}n_i$:

$$GA_1(HS) = \frac{8\sqrt{6} + 5}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{8\sqrt{6} - 25}{5} \quad (10)$$

In similar way the formula for calculating GA_1 of phenylenes is obtained:

$$GA_1(PH) = \frac{8\sqrt{6} + 20}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{8\sqrt{6} - 10}{5}. \quad (11)$$

Combining the Eqs. (10) and (11) we get linear relation between GA_1 of phenylene and its hexagonal squeeze:

$$GA_1(PH) - GA_1(HS) = 3(h - 1).$$

2.2.4. GA_1 index of $TUC_4C_8(S)$ nanotubes

Since the discovery of buckminsterfullerene [43] and latter of nanotubes [44], the investigation of nanomolecules, both by experimental and theoretical chemists, has been intensively conducted. Nowadays, there is a vast number of papers and several books dealing with these molecules. Theoreticians predicted many structures of fullerenes, nanotubes, nanotoruses, . . . , expecting to be synthesized in the future [45].

One class of such nanomolecules are the $TUC_4C_8(S)$ nanotubes. There are several papers where various topological indices of these molecules were investigated [46–52]. In Fig. 5 is shown the structure of this type of nanotubes.

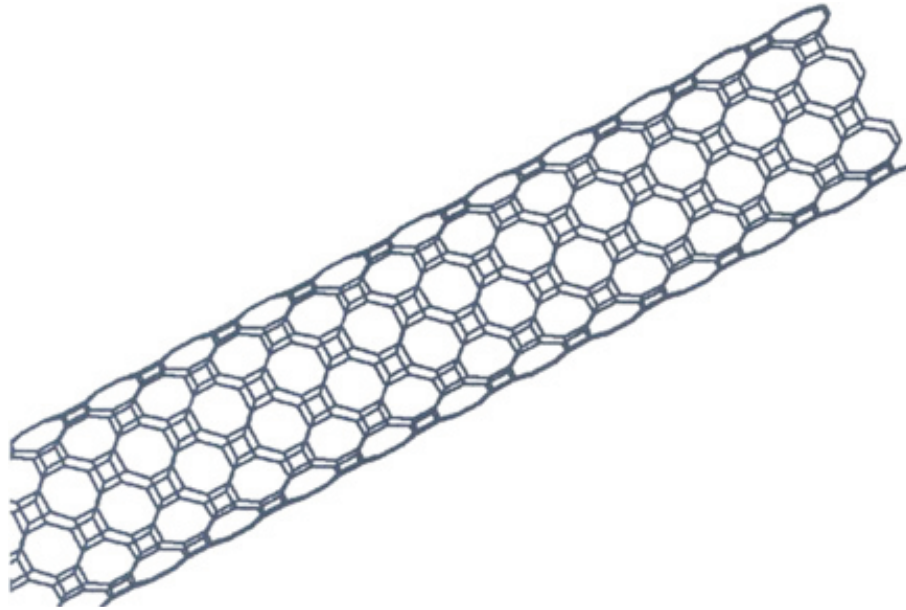


Figure 5. A $TUC_4C_8(S)$ nanotube

In the paper [53], thje authors found exact formulas for calculation of the GA_1 index of the two-dimensional lattice of the $TUC_4C_8(S)$ graph ($KTUC[p, q]$), $TUC_4C_8(S)$ nanotube ($GTUC[p, q]$), and $TUC_4C_8(S)$ nanotorus ($HTUC[p, q]$) in terms of parameters p and q . The two-dimensional lattice of the $TUC_4C_8(S)$ graph is tessellated by alternating squares (C_4) and octagons (C_8) and it is shown in Fig. 6.

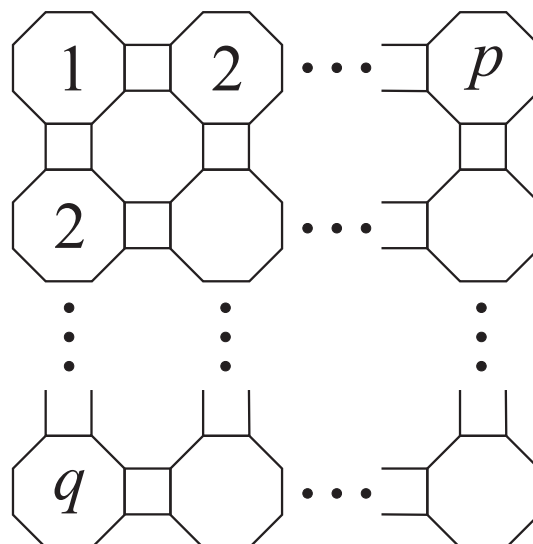


Figure 6. A $TUC_4C_8(S)$ lattice, where p and q denotes the number of octagons in rows and columns, respectively.

The same authors obtained for two-dimensional lattice of the $TUC_4C_8(S)$ graph ($KTUC[p, q]$) the following formula:

$$GA_1(KTUC[p, q]) = 12pq + \left(\frac{8\sqrt{6}}{5} - 6 \right) (q - p) + 8 - \frac{16\sqrt{6}}{5} .$$

For $TUC_4C_8(S)$ nanotube ($GTUC[p, q]$), they found the following expression:

$$GA_1(GTUC[p, q]) = 12pq + \left(\frac{8\sqrt{6}}{5} - 6 \right) p .$$

Since nanotoruses are 3-regular graphs, then the GA_1 index is equal to the number of edges. In this case, the first geometric–arithmetic index is simply

$$GA_1(HTUC[p, q]) = 12pq .$$

3. The Second Geometric–arithmetic Index

The “*second geometric–arithmetic index*” has been put forward very recently as a continuation of research on geometric–arithmetic indices [9]. It is also based on Eq. (1), and its definition is given by Eq. (5).

3.1. GA_2 as a tool for QSAR/QSPR researches

The GA_2 index was correlated with the already established GA_1 index in the case of octanes. In Table 4 are given values of GA_1 and GA_2 indices for octane isomers. Fig. 7 shows the correlation between these two indices.

By a superficial inspection of the correlation, it appears to be linear but weak. The data points **15**, **13**, **5**, **9**, **2**, and **1** form an almost perfect straight line with increasing slope. If we denote the number of quaternary and tertiary carbon atoms by n_4 and n_3 , we may immediately check that for these isomers (n_4, n_3) is equal to $(2, 0)$, $(1, 1)$, $(1, 0)$, $(0, 2)$, $(0, 1)$, and $(0, 0)$, respectively. This shows that both GA_1 and GA_2 are increasing functions of the extent of branching of the molecular skeleton. It is worth noting that the molecules **15**, **13**, **5**, **9**, and **2** are all branched at the very end of their carbon–atom chains.

#	octanes	GA_1	GA_2	GA_3
1	n-octane	6.88562	5.99142	4.37633
2	2-methyl heptane	6.65466	5.78683	3.63097
3	3-methyl heptane	6.71124	5.68461	3.43352
4	4-methyl heptane	6.71124	5.65286	3.37633
5	2,2-dimethyl hexane	6.28562	5.48002	2.68817
6	3,3-dimethyl hexane	6.37124	5.34605	2.43352
7	2,3-dimethyl hexane	6.52068	5.44827	2.63097
8	2,4-dimethyl hexane	6.48027	5.48002	2.68817
9	2,5-dimethyl hexane	6.42369	5.58224	2.88562
10	3,4-dimethyl hexane	6.57726	5.37780	2.49071
11	2,3,4-trimethyl pentane	6.33013	5.24368	1.88562
12	2,2,3-trimethyl pentane	6.17837	5.17321	1.74536
13	2,2,4-trimethyl pentane	6.05466	5.27543	1.94281
14	2,3,3-trimethyl pentane	6.20741	5.14146	1.68817
15	2,2,3,3-tetramethyl butane	5.80000	4.96863	1.00000
16	3-ethyl-2-methyl pentane	6.57726	5.34605	2.43352
17	3-ethyl-3-methyl pentane	6.45685	5.24383	2.23607
18	3-ethyl hexane	6.76781	5.55064	3.17888

Table 4. GA_1 , GA_2 , and GA_3 indices of all 18 octane isomers

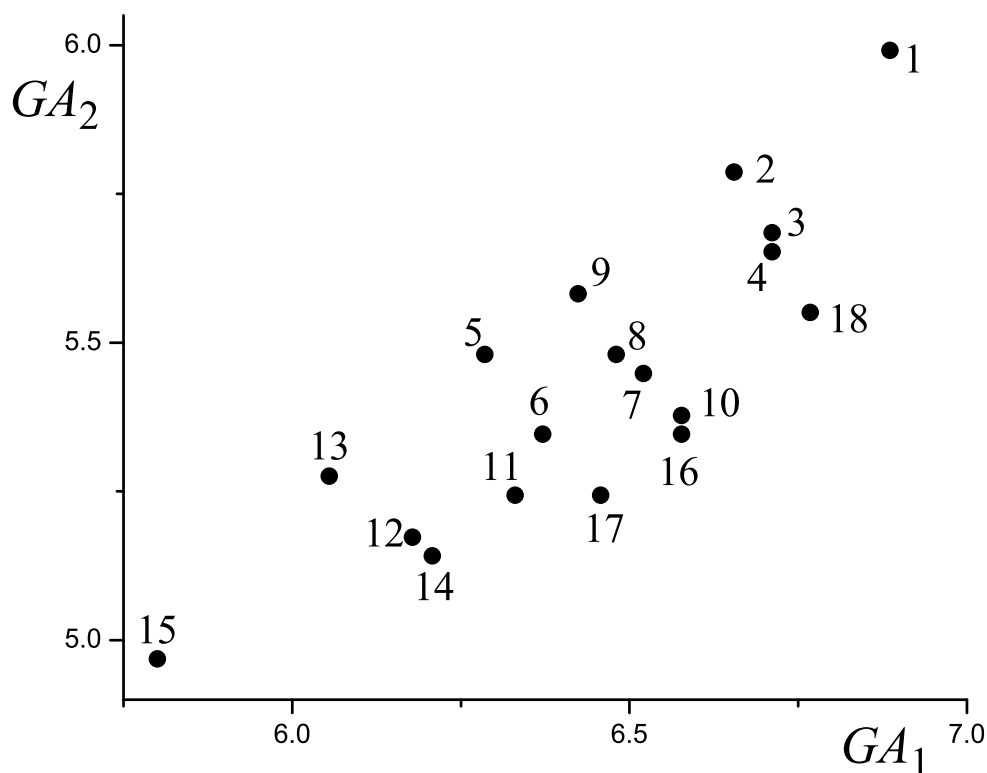


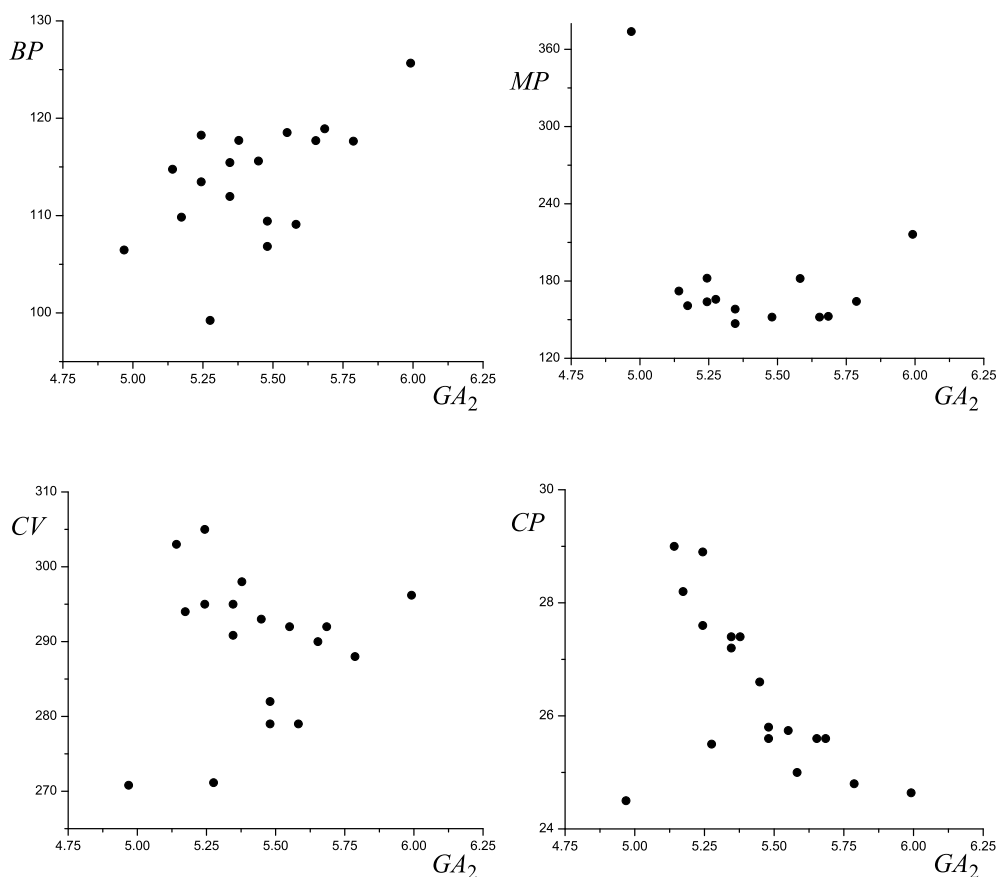
Figure 7. Correlations between GA_1 and GA_2 of octanes; the numbering of the data points corresponds to Table 4.

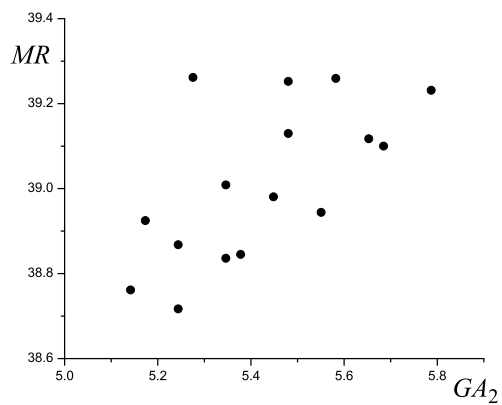
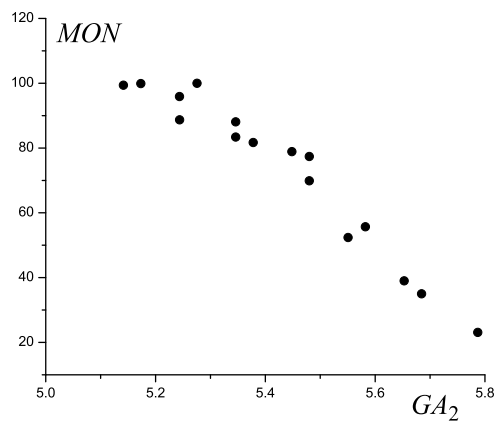
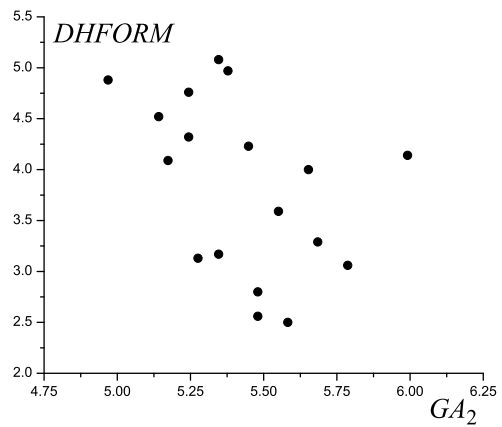
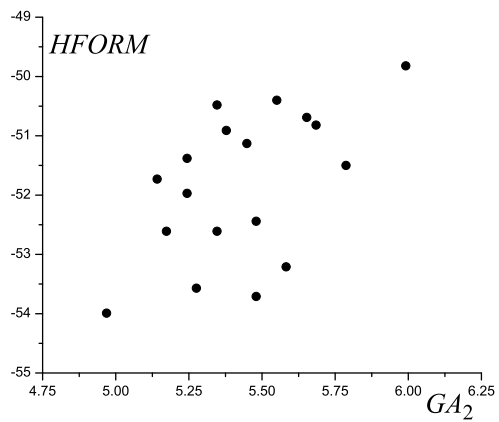
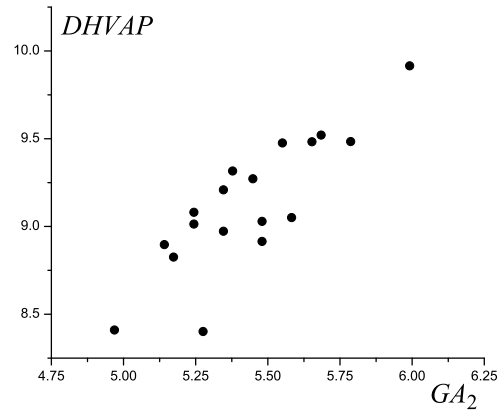
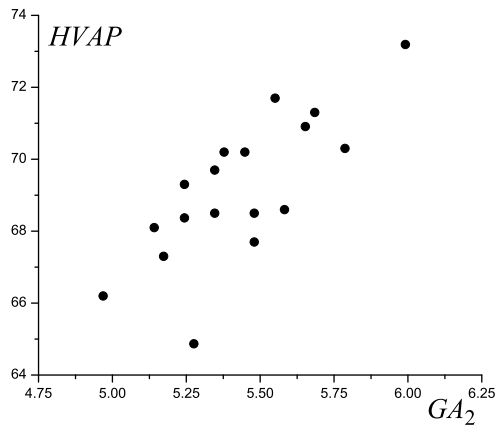
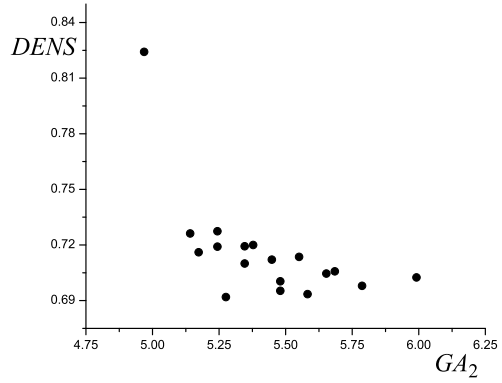
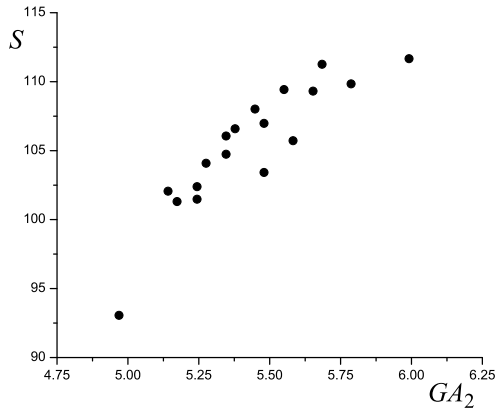
A detailed examination of Fig. 7 reveals that the data points are grouped into several clusters. By direct checking it is verified that each cluster corresponds to a particular choice of (n_4, n_3) . The apparent outlier **11** pertains to 2,3,4-trimethyl pentane, the only octane isomer for which $(n_4, n_3) = (0, 3)$.

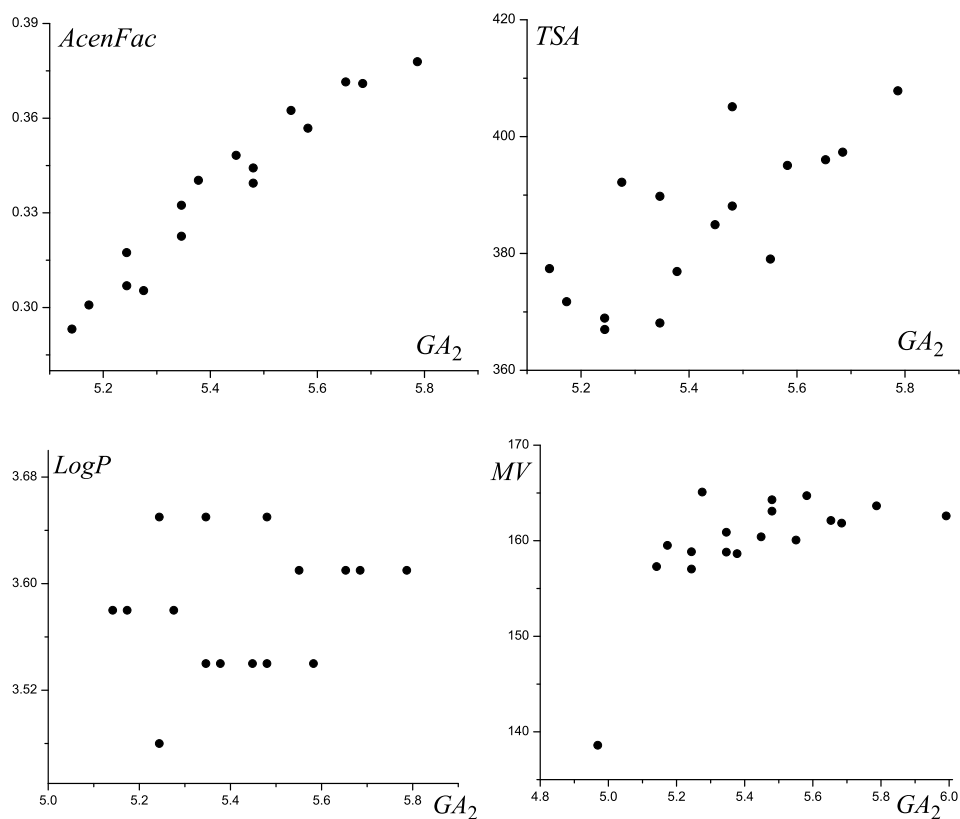
Thus, the isomers belonging to the same cluster are those similarly branched. Within each such cluster (provided that there are two or more data points), the proportionality between GA_1 and GA_2 is inverse. For instance, the data points **7, 8, 9, 10**, and **16**, all pertaining to $(n_4, n_3) = (0, 2)$, lie nearly on a straight line with decreasing slope.

The above described relations between GA_1 and GA_2 , which hold not only for octanes, but for all chemical trees, indicate that these indices depend in the same way on one structural feature (namely, on branching), but have a different dependence on some other details of molecular structure. This gives hope that GA_1 and GA_2 will both be simultaneously applicable in QSPR and QSAR studies.

Similarly as in sub-section 2.1. we are showing the correlations between the GA_2 index and 16 physico-chemical properties of octanes.







From the above figures it can be seen that there exists a useful linear correlation between GA_2 and only four physico-chemical properties, i. e., entropy (S), standard enthalpy of vaporization (DH_{VAP}), motor octane number (MON), and acentric factor ($Acenfac$). The respective correlation coefficients are given in Table 5.

Physico-chemical property	Correlation coefficient (R)
S	0.890
DH_{VAP}	0.843
MON	0.968
$AcenFac$	0.973

Table 5.

3.2. Mathematical properties of GA_2

In this section we are concerned with connected simple graphs with n vertices and m edges.

3.2.1. Lower and upper bounds for GA_2

Lower and upper bounds of GA_2 index for bipartite graphs were communicated in [9, 13]:

$$\frac{2(n-1)^{3/2}}{n} = GA_2(S_n) \leq GA_2(G) = GA_2(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) \leq \begin{cases} n^2/4 & \text{if } n \text{ is even} \\ (n^2-1)^{3/2}/4n & \text{if } n \text{ is odd} \end{cases}.$$

Furthermore, the star S_n has minimum second geometric–arithmetic index among all connected graphs. This comes from the following inequality that is true for all connected graphs [9]:

$$GA_2(G) \geq \frac{2m\sqrt{n-1}}{n}. \quad (12)$$

Equality in (12) is achieved if and only if $G \cong S_n$ (i. e., G is the star).

Other lower and upper bounds of GA_2 index are in terms of vertex Padmakar–Ivan index and Szeged index.

The vertex Padmakar–Ivan index (PI_v) [11] has been introduced recently inspired by the definition of the “original” PI index which already had many applications in chemistry (e.g. see [54] and references cited therein).

$$PI_v(G) = \sum_{uv \in E(G)} [n_u(e) + n_v(e)]$$

The definition of $n_u(e)$ and $n_v(e)$ is given by Eq. (3). More details about vertex PI index can be found in [55–58].

The Szeged index was introduced in 1994 as an extension to all graphs of the well-known Wiener’s formula for the calculation of the Wiener index of trees [10]:

$$Sz(G) = \sum_{uv \in E(G)} n_u(e) \cdot n_v(e)$$

where n_u and n_v are defined by Eq. (3). This index was extensively studied in past fifteen years. Mathematical properties of the Szeged index are outlined in a number of papers; for a review see [59]. Chemical applications of the Szeged index were presented in the book [54].

Among all connected graphs the following inequality is true [9]:

$$GA_2(G) \leq \frac{1}{2} PI_v(G)$$

where equality holds if and only if G is the complete graph.

In the same paper it was shown that for all connected graphs with m edges

$$GA_2(G) \leq \sqrt{m Sz(G)} \quad (13)$$

where equality holds if and only if the G is the complete graph.

In the paper [13] a similar inequality was reported, applicable to bipartite connected graphs with n vertices and m edges:

$$GA_2(G) \leq \frac{2}{n} \sqrt{m Sz(G)}$$

with equality if and only if $n_u n_v$ is a constant for any $uv \in E(G)$.

In [9] was also proven another upper bound for GA_2 index for all connected graphs with m edges in terms of the Szeged index:

$$GA_2(G) \leq \sqrt{Sz(G) + m(m-1)} \quad (14)$$

with equality if and only if $G \cong K_n$.

For the complete graph, the inequalities (13) and (14) are equivalent. For all other connected graphs, the upper bound (14) is better than (13).

In the same paper a lower bound for the GA_2 index for connected graphs with n vertices and m edges in terms of the Sz index was established:

$$GA_2(G) \geq \frac{2}{n} \sqrt{Sz(G) + m(m-1)}. \quad (15)$$

Equality in (15) is attained if and only if $G \cong K_2$.

For the complete graph with two vertices, inequalities (15) and (12) are equivalent. For all other connected graphs the lower bound (12) is better than (15).

3.2.2. Extremal values of the GA_2 index of trees

The trees with extremal values of GA_2 index are presented in the paper [9]. There the following was shown:

$$GA_2(S_n) \leq GA_2(T) \leq GA_2(P_n)$$

where T is any n -vertex tree. If $T \not\cong S_n, P_n$, then the above inequalities are strict. Thus, the tree with smallest GA_2 index is the star, and the path has the greatest value of GA_2 .

4. The Third Geometric–arithmetic Index

The “*third geometric–arithmetic index*” (GA_3) is at the present moment (December 2009) the last index belonging to the GA class. It has been introduced in the paper [13] and is defined by Eq. (6). Some of its properties are discussed in this section.

4.1. GA_3 as a tool for QSAR/QSPR researches

In order to check if the GA_3 index is a possible tool for QSAR/QSPR researches, we first examine its correlation with other indices from a GA class.

The correlation between the GA_3 index and the GA_1 and GA_2 indices are studied in the case of octanes. The values of those three indices are given in Table 4, whereas Figs. 8 and 9 show these correlations.

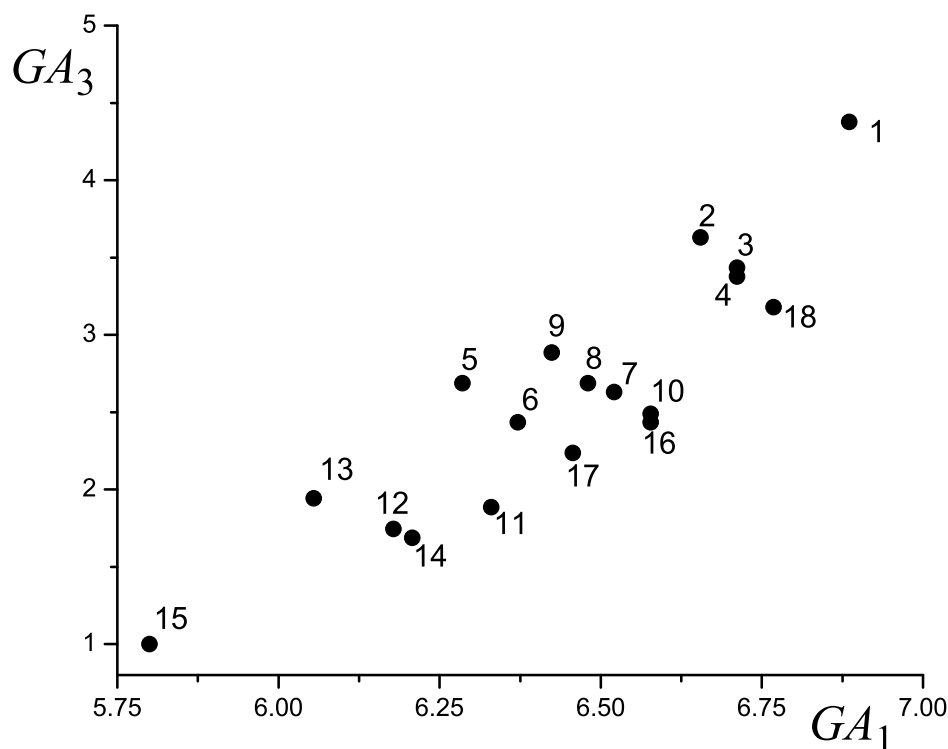


Figure 8.

Comparing Figs. 7 and 8 it is evident that they are qualitatively very similar. Therefore, all conclusions derived for the correlation between GA_1 and GA_2 indices are applicable also in this case. Briefly, there exists a weak linear correlation between GA_1 and GA_3 , and the clustering of the points in Fig. 8 is caused by the number of quaternary (n_4) and tertiary (n_3) carbon atoms. It can be seen that both the GA_1 and GA_3 indices are increasing functions of the extent of branching in acyclic molecules.

The correlation between GA_2 and GA_3 indices is shown in Fig. 9.

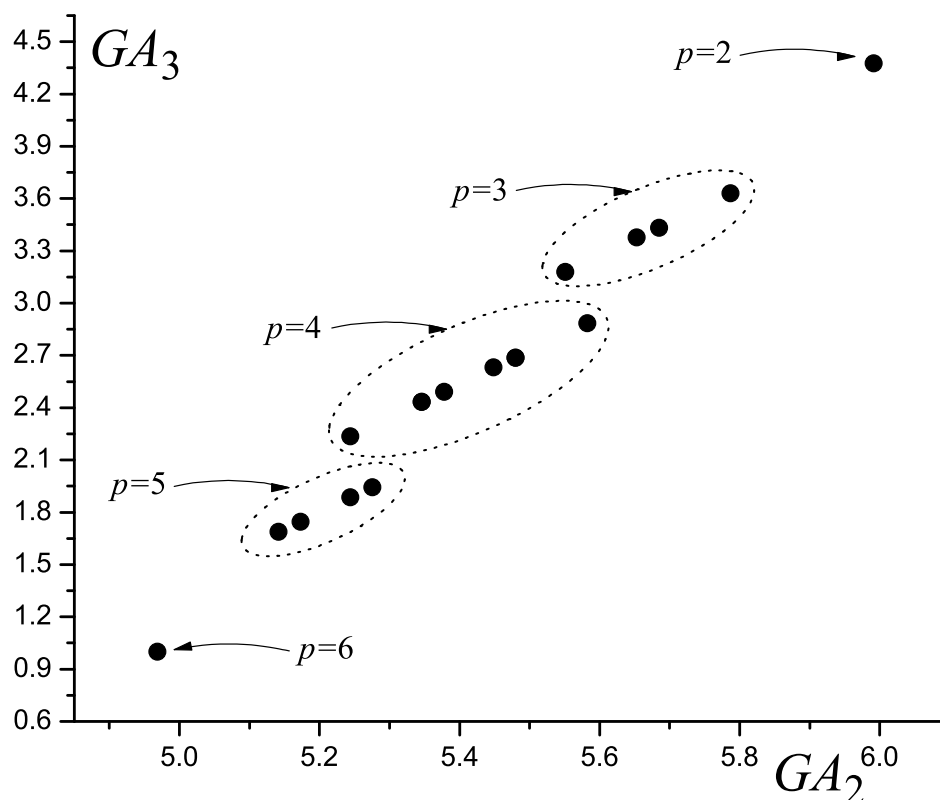


Figure 9.

By a superficial glance at Fig. 9 it appears that between GA_2 and GA_3 there exists a reasonably good linear correlation ($R = 0.989$). In addition, it is noticed that all points are grouped into few nearly parallel lines. By inspecting the data more carefully we found that the points are clustered by the number of pendent vertices (p) in a chemical tree (i. e., by the number CH_3 groups in the corresponding alkanes). The octanes belonging to each line as well as the parameters of lines and correlation coefficients are given in Table 6.

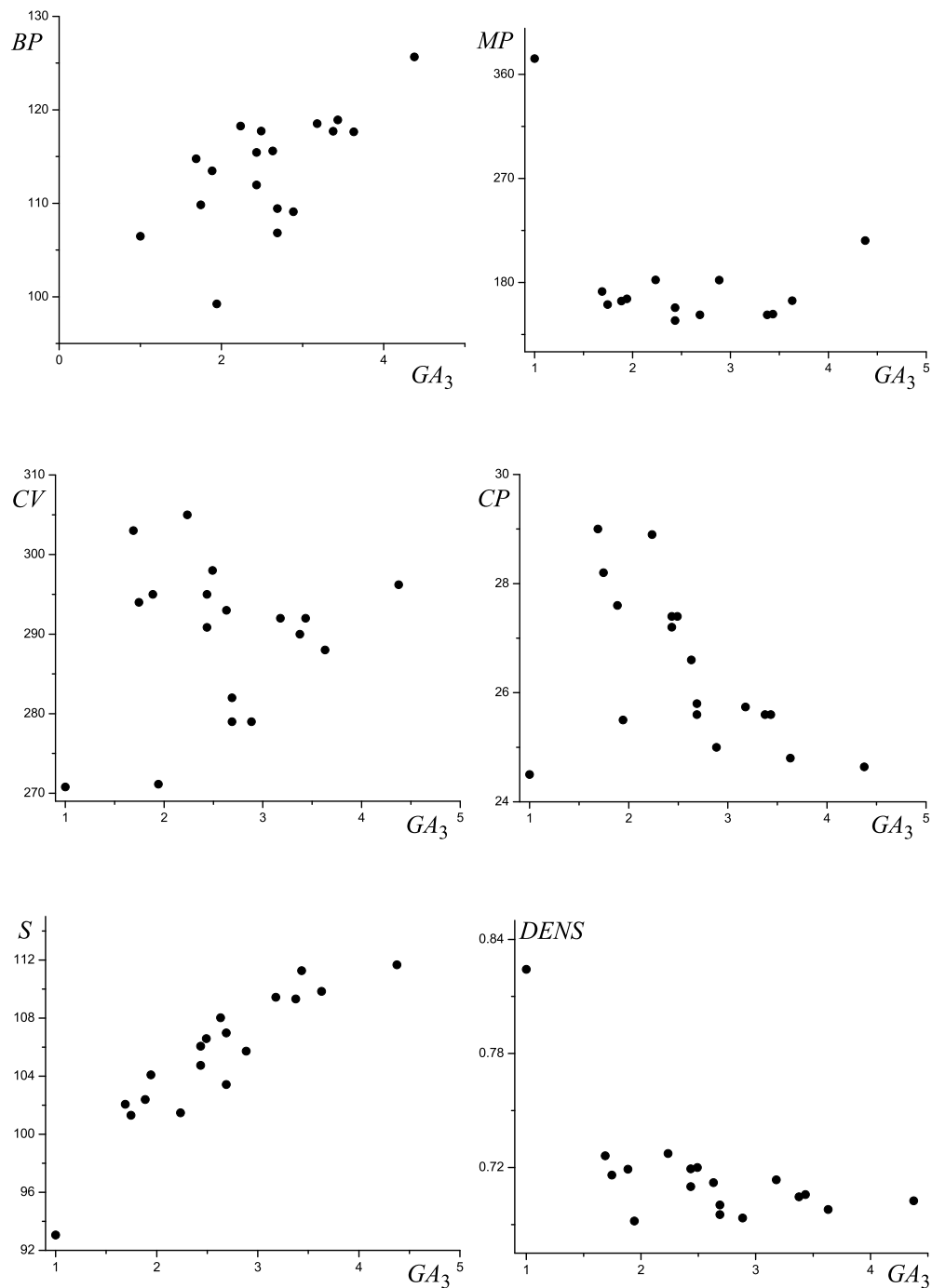
p	Molecule*	$a \pm \Delta a$	$b \pm \Delta b$	R
2	1	—	—	—
3	2, 3, 4, 18	1.910 ± 0.010	-7.43 ± 0.06	0.99997
4	5, 6, 7, 8, 9, 10, 16, 17	1.917 ± 0.006	-7.82 ± 0.03	0.99997
5	11, 12, 13, 14	1.920 ± 0.030	-8.20 ± 0.10	0.99982
6	15	—	—	—

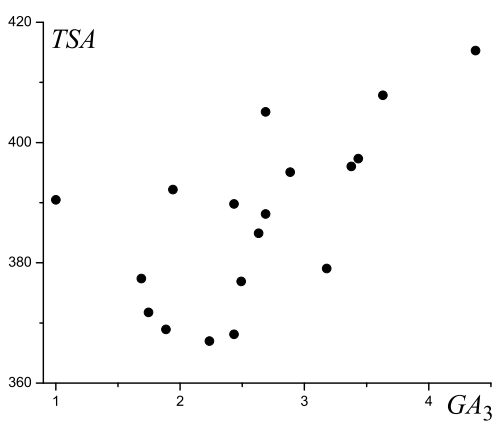
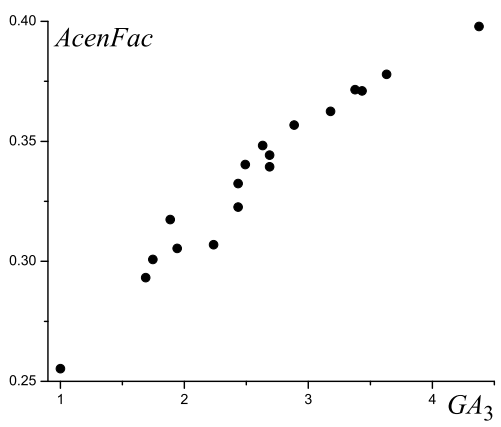
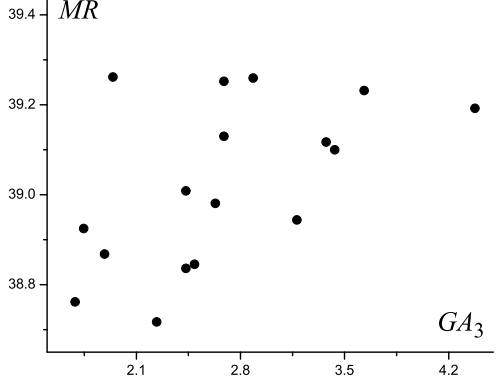
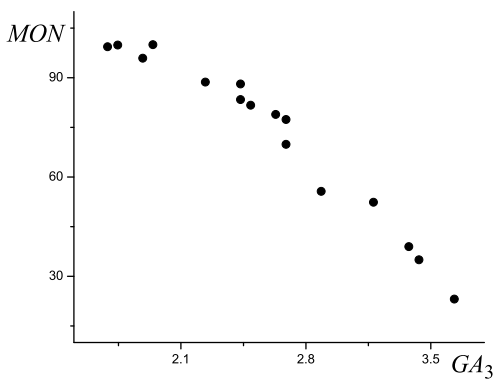
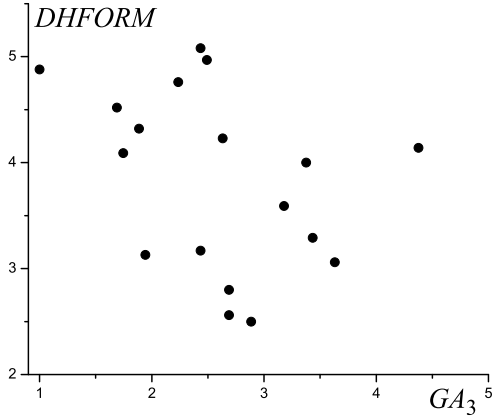
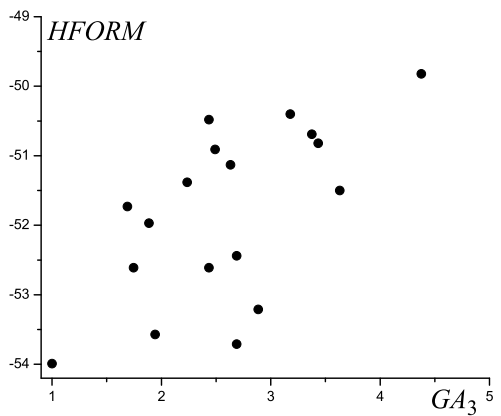
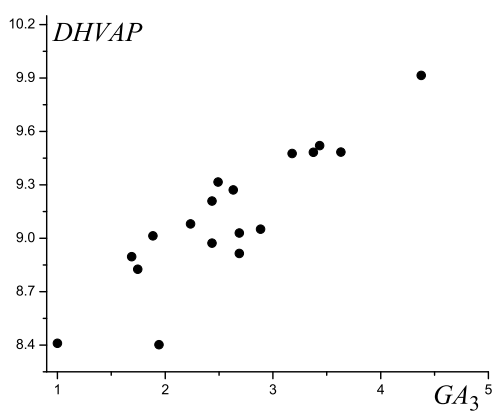
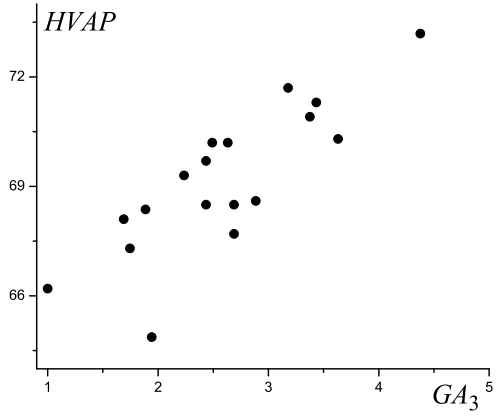
* The given numbers correspond to numbering of octanes in Table 4.

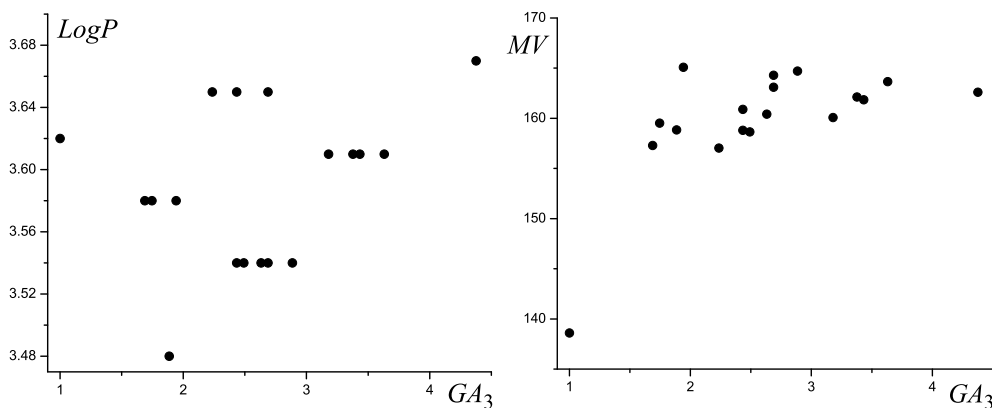
Table 6. p is the number of pendent vertices; a and Δa are the slope of the line and the respective absolute error; b and Δb are the intercept of the line and the respective absolute error; R is the correlation coefficient.

These subtle differences of dependence on some structural properties gives us hope that the GA_3 index may be applicable in QSAR/QSPR investigations.

In the following pictures are given the correlations between the GA_3 index and the 16 physico-chemical properties of octane isomers, same as those used in the previous sections.







From the above figures it can be seen that there exist useful linear correlation ($R \geq 0.8$) between GA_3 and five physico-chemical properties of octanes, namely entropy (S), enthalpy of vaporization ($HVAP$), standard enthalpy of vaporization ($DHVAP$), motor octane number (MON), and acentric factor ($AcenFac$). Without any further discussion, the corresponding correlation coefficients are given in Table 7.

Physico-chemical property	Correlation coefficient (R)
S	0.909
$HVAP$	0.828
$DHVAP$	0.890
MON	0.970
$AcenFac$	0.975

Table 7.

Comparing the R 's from Table 7 with those presented in Table 5 (for the GA_2 index) it can be concluded that the GA_3 index gives somewhat better predictions of the presented properties than GA_2 .

4.2. Mathematical properties of GA_3

As in the previous sections on mathematical properties of the GA indices, we are going to consider only simple connected graphs. By $S_{p,q}$, for $p, q \geq 2$, will be denoted the $(p+q)$ -vertex tree formed by adding an edge between centers of the stars S_p and S_q . The tree $T_n(\Delta)$ is formed by attaching $\Delta - 1$ pendent vertices to a terminal vertex of the path $P_{n-\Delta+1}$, where $2 \leq \Delta \leq n - 1$. The tree $T(n, 2)$ is obtained from the path (P_{n-1}) by attaching a pendent vertex to its vertex at distance 2 from a terminal vertex.

The edge–Szeged index has been put forward recently. It is defined as [14]

$$Sz_e(G) = \sum_{uv \in E(G)} m_u \cdot m_v .$$

For more results about the edge–Szeged index consult the papers [60–65].

4.2.1. Lower and upper bounds for GA_3

For all connected graphs with n vertices the following inequality holds [13]:

$$0 = GA_3(S_n) \leq GA_3(G) \leq GA_3(K_n) = \frac{n(n-1)}{2}$$

In the same paper, some more bounds were obtained for GA_3 for simple connected graphs with $m \geq 2$ edges in terms of the edge–Szeged index:

$$\frac{2}{m-1} \sqrt{Sz_e(G)} \leq GA_3(G) \leq \sqrt{Sz_e(G) + m(m-1)}$$

The left equality is achieved if and only if $G \cong S_{m+1}$ or $G \cong S_{p,m+1-p}$ with $2 \leq p \leq \lfloor (m+1)/2 \rfloor$. The right equality is attained if and only if the G is the triangle or the quadrangle.

4.2.2. Extremal values of the GA_3 index of trees

In [13] the trees with minimum and maximum values of GA_3 index were determined. There the following inequality was obtained:

$$GA_3(S_n) \leq GA_3(T) \leq GA_3(P_n) .$$

In the same work also the trees with second, third, fourth, and fifth minimum GA_3 index were characterized.

The unique tree with the second minimum GA_3 index is $S_{2,n-2}$ for $n \geq 4$ and

$$GA_3(S_{2,n-2}) = \frac{2\sqrt{n-3}}{n-2} .$$

For $n \geq 6$ vertices $S_{3,n-3}$ is the unique tree with the third minimum GA_3 index equal to

$$GA_3(S_{3,n-3}) = \frac{2\sqrt{2(n-4)}}{n-2} .$$

For trees with $n \geq 8$ vertices $S_{4,n-4}$ is the tree with fourth smallest GA_3 index, equal to

$$GA_3(S_{4,n-4}) = \frac{2\sqrt{3(n-5)}}{n-2} .$$

The tree with the fifth minimum GA_3 index with $n \geq 10$ vertices is $S_{5,n-5}$ and

$$GA_3(S_{5,n-5}) = \frac{2\sqrt{4(n-6)}}{n-2}.$$

As it was previously stated, the tree with maximum GA_3 index among all n -vertex trees is the path P_n . Its GA_3 -values can be calculated as:

$$GA_3(P_n) = \frac{2}{n-2} \sum_{i=1}^{n-3} \sqrt{i(n-2-i)}.$$

The tree with the second maximum GA_3 index can be formed by attaching two pendent vertices to an end-vertex of the path P_{n-2} . Let us label this tree by $T(n, 1)$. Its GA_3 -value is equal to

$$GA_3(T(n, 1)) = \frac{2}{n-2} \sum_{i=1}^{n-4} \sqrt{i(n-2-i)}.$$

Among the n -vertex trees with $n \geq 6$, $T(n, 2)$ is the unique tree with the third maximum GA_3 -value, equal to

$$GA_3(T(n, 2)) = \frac{2}{n-2} \left[\sum_{i=1}^{n-3} \sqrt{i(n-2-i)} - 2(n-4) \right].$$

Let G be a tree with n vertices and maximum vertex degree Δ , where $2 \leq \Delta \leq n-1$. Then

$$GA_3(G) \leq \frac{2}{n-2} \sum_{i=1}^{n-3} n - \Delta - 1 \sqrt{i(n-2-i)}$$

where equality is attained if and only if $G \cong T_n(\Delta)$.

5. Conclusion

In this survey, probably all results about GA indices are outlined. We believe that in the future the research on this class of indices will continue. The results obtained so far give us hope that the GA class of indices has a future in QSAR/QSPR researches.

Acknowledgement: The authors thank the Serbian Ministry of Science for support, through Grant no. 144015G.

References

- [1] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [2] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [3] I. Gutman, The energy of a graph, *Ber. Math.-Statist. Sect. Forschungsz. Graz* **103** (1978) 1–22.
- [4] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.
- [5] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
- [6] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [7] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Japan* **44** (1971) 2332–2339.
- [8] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.
- [9] G. Fath-Tabar, B. Furtula, I. Gutman, A new geometric-arithmetic index, *J. Math. Chem.* in press.
- [10] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes New York* **27** (1994) 9–15.
- [11] M. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Vertex and edge *PI* indices of Cartesian product of graphs, *Discr. Appl. Math.* **156** (2008) 1780–1789.
- [12] F. Buckley, F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, 1990.
- [13] B. Zhou, I. Gutman, B. Furtula, Z. Du, On two types of geometric-arithmetic index, *Chem. Phys. Lett.* **482** (2009) 153–155.
- [14] I. Gutman, A. R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* **81** (2008) 263–266.
- [15] P. V. Khadikar, On a novel structural descriptor *PI*, *Nat. Acad. Sci. Lett.* **23** (2000) 113–118.
- [16] X. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

- [17] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.
- [18] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.
- [19] Y. Yuan, B. Zhou, N. Trinajstić, On geometric–arithmetic index, *J. Math. Chem.* in press.
- [20] K. C. Das, On geometric–arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.* in press.
- [21] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Am. Math. Monthly* **63** (1956) 175–177.
- [22] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd revised ed. 1992.
- [23] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1988.
- [24] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1989.
- [25] M. Vöge, A. J. Guttmann, I. Jensen, On the number of benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **42** (2002) 456–466.
- [26] TRC Thermodynamic Tables – Hydrocarbons; Thermodynamic Research Center, The Texas A & M University System: College Station, TX, 1987.
- [27] K. P. C. Vollhardt, The phenylenes, *Pure Appl. Chem.* **65** (1993) 153–156.
- [28] K. P. C. Vollhardt, D. L. Mohler, The phenylenes: Synthesis, properties, and reactivity, in: B. Halton (Ed.), *Advances in Strain in Organic Chemistry*, Vol. 5, JAI Press, London, 1996, pp. 121–160.
- [29] N. Trinajstić, T. G. Schmalz, T. P. Živković, S. Nikolić, G. E. Hite, D. J. Klein, W. A. Seitz, [*N*]-phenylenes: A theoretical study, *New J. Chem.* **15** (1991) 27–31.
- [30] M. Baumgarten, F. Dietz, K. Müllen, S. Karabunarliev, N. Tyutyulkov, Energy spectral of infinite phenylenes, *Chem. Phys. Lett.* **221** (1994) 71–74.
- [31] I. Gutman, B. Furtula, A Kekulé structure basis for phenylenes, *Journal of Molecular Structure (Theochem)* **770** (2006) 67–71.
- [32] I. Gutman, Easy method for the calculation of the algebraic structure count of phenylenes, *J. Chem. Soc. Faraday Trans.* **89** (1993) 2413–2416.
- [33] I. Gutman, S. J. Cyvin, J. Brunvoll, Enumeration of the isomers of phenylenes, *Monatsh. Chem.* **125** (1994) 887–894.

- [34] I. Gutman, A regularity for the total π -electron energy of phenylenes, *MATCH Commun. Math. Chem.* **31** (1994) 99–110.
- [35] I. Gutman, S. Marković, A. Stajković, S. Kamidžorac, Correlations between π -electron properties of phenylenes and their hexagonal squeezes, *J. Serb. Chem. Soc.* **61** (1996) 873–879.
- [36] I. Gutman, S. Marković, L. Popović, Z. Spalević, L. Pavlović, The relation between the Wiener indices of phenylenes and their hexagonal squeezes, *J. Serb. Chem. Soc.* **62** (1997) 207–210.
- [37] L. Pavlović, I. Gutman, Wiener numbers of phenylenes: An exact result, *J. Chem. Inf. Comput. Sci.* **37** (1997) 355–358.
- [38] I. Gutman, S. Klavžar, Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes, *ACH – Models Chem.* **135** (1998) 45–55.
- [39] B. Furtula, I. Gutman, Ž. Tomović, A. Vesel, I. Pesek, Wiener-type topological indices of phenylenes, *Indian J. Chem.* **41A** (2002) 1767–1772.
- [40] J. Rada, O. Araujo, I. Gutman, Randić index of benzenoid systems and phenylenes, *Croat. Chem. Acta* **74** (2001) 225–235.
- [41] B. Furtula, I. Gutman, Assessing the distribution of π -electrons into rings of phenylenes, *Indian J. Chem.* **45A** (2006) 1977–1980.
- [42] B. Furtula, I. Gutman, Energy and Estrada index of phenylenes, *Indian J. Chem.* **47A** (2008) 220–224.
- [43] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, C₆₀: buckminsterfullerene, *Nature* **318** (1985) 162–163.
- [44] S. Iijima, Helical microtubules of graphitic carbon, *Nature* **354** (1991) 56–58.
- [45] M. V. Diudea, C. L. Nagy, *Periodic nanostructures*, Springer Netherlands, Dordrecht, 2007.
- [46] A. R. Ashrafi, A. Loghman, Padmakar–Ivan index of $TUC_4C_8(S)$ nanotubes, *J. Comput. Theor. Nanosci.* **3** (2006) 378–381.
- [47] A. Heydari, B. Taeri, Wiener and Schultz indices of $TUC_4C_8(S)$ nanotubes, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 665–676.
- [48] A. Iranmanesh, Y. Pakraves, Detour index of $TUC_4C_8(S)$ nanotube, *Ars Combin.* **84** (2007) 247–254.
- [49] A. Iranmanesh, A. S. Kafrani, Computation of the first edge–Wiener index of $TUC_4C_8(S)$ nanotube, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 311–354.

- [50] A. Heydari, B. Taeri, Szeged index of $TUC_4C_8(S)$ nanotubes *Eur. J. Combin.* **30** (2009) 1134–1141.
- [51] M. Arezoomand, B. Taeri, A mathematical model for $TUC_4C_8(S)$ nanotubes and their symmetry, *J. Geom. Phys.* **59** (2009) 1168–1174.
- [52] S. Xu, H. Zhang, Hosoya polynomials of $TUC_4C_8(S)$ nanotubes, *J. Math. Chem.* **45** (2009) 488–502.
- [53] M. Ghorbani, M. Jalali, Computing a new topological index of nano structures, *Dig. J. Nanomater. Bios.* **4** (2009) 681–685.
- [54] M. V. Diudea, M. S. Florescu, P. V. Khadikar, *Molecular Topology and Its Applications*, EfiCon Press, Bucharest, 2006.
- [55] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, A matrix method for computing Szeged and vertex PI indices of join and composition of graph, *Lin. Algebra Appl.* **429** (2008) 2702–2709.
- [56] M. J. Nadjafi–Arani, G. H. Fath–Tabar, A. R. Ashrafi, Extremal graphs with respect to the vertex PI index, *Appl. Math. Lett.* **22** (2009) 1838–1840.
- [57] M. Mogharrab, H. Maimani, A. R. Ashrafi, A note on the vertex PI index of graphs, *J. Adv. Math. Studies* **2** (2009) 53–56.
- [58] T. Mansour, M. Schork, The vertex PI index and Szeged index of bridge graphs, *Discr. Appl. Math.* **157** (2009) 1600–1606.
- [59] I. Gutman, A. A. Dobrynin, The Szeged index – a success story, *Graph Theory Notes New York* **34** (1998) 37–44.
- [60] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, I. Gutman, The edge Szeged index of product graphs, *Croat. Chem. Acta* **81** (2008) 277–281.
- [61] A. R. Ashrafi, M. Mirzagar, PI , Szeged and edge Szeged indices of an infinite family of nanostar dendrimers, *Indian J. Chem.* **47A** (2008) 538–541.
- [62] E. Chiniforooshan, B. Wu, Maximum values of Szeged index and edge–Szeged index of graphs, *El. Notes Discr. Math.* **34** (2009) 405–409.
- [63] K. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, S. G. Wagner, Some new results on distance–based graph invariants, *Eur. J. Combin.* **30** (2009) 1149–1163.
- [64] D. Vukičević, Note on the graphs with the greatest edge–Szeged index, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 673–681.
- [65] X. Cai, B. Zhou, Edge Szeged index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 133–144.