

# Survey on Geometric–Arithmetic Indices of Graphs

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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 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 [42, 43, 81]. They can be classified by the structural properties of the graphs used for their calculation. Hence, the probably best known and most widely used Wiener index [12, 90, 93] is based on topological distance of vertices in the respective graph, the Hosoya index [53, 66] is calculated by counting non-incident edges in a graph, the energy [31, 35, 46] and the Estrada index [23, 94] are based on the spectrum of the graph, the Randić connectivity index [22, 79] and the Zagreb group indices [10, 49, 69] 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 [24]:

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

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  $v$  connected by an edge). Summation goes over all edges in the respective graph  $G$ . Three members of  $GA$  group topological indices have been put forward up to now.

The first member [87] 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 calling  $GA_1$  the “*first geometric–arithmetic index*”.

Another member of this class, denoted by  $GA_2$ , 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 [79],  $GA_2$  is constructed in such a manner that it is related with the Szeged [33] and vertex Padmakar–Ivan [62] 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 [5], 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

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

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,

$$n_u(e, G) + n_v(e, G) = n \tag{4}$$

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

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

Currently, the last introduced topological index belonging to the  $GA$  class is the so-called the “*third geometric–arithmetic index*”, denoted as  $GA_3$  [96]. In order to define it, 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

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

Similarly to  $GA_2$ , the *third geometric–arithmetic index* is defined so as to be related to the recently introduced edge Szeged ( $Sz_e$ ) index [36] and edge Padmakar–Ivan ( $PI_e$ ) index [60].

## 2. Is the Ratio between Geometric and Arithmetic Means the Right Choice?

Statistical researches are practically unimaginable without using the means. That is why the means attracted mathematicians over the centuries. The results on means are numerous and several books have appeared collecting them (see for example [50, 72]).

The majority of people is familiar with the well-known arithmetic and geometric means. However, the number of means is practically infinite, and a general formula for their calculation is as follows:

$$M_p = M_p(x_1, x_2, \dots, x_n) = \left( \frac{1}{n} \sum_{i=1}^n (x_i)^p \right)^{1/p}. \tag{7}$$

It can be easily seen that arithmetic mean is attained when  $p = 1$ , and geometric mean when  $p = 0$ . Therefore, the definition of geometric–arithmetic indices can be rewritten in the following manner:

$$GA_{general}(G) = \sum_{uv \in E(G)} \frac{M_0(Q_u Q_v)}{M_1(Q_u Q_v)}.$$

Taking into mind Eq. (7), it is natural asking ourselves the question pointed out in the title of this section. In the rest of this section, this problem will be analyzed for all three geometric–arithmetic indices.

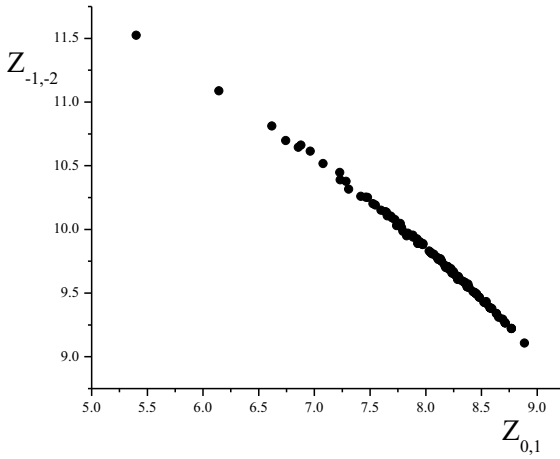
In order to determine if the ratio between geometric and arithmetic means, in the case of the first geometric–arithmetic index, is the right choice, an exhaustive computer research was performed [20].

Let us define a general class of indices based on means as follows:

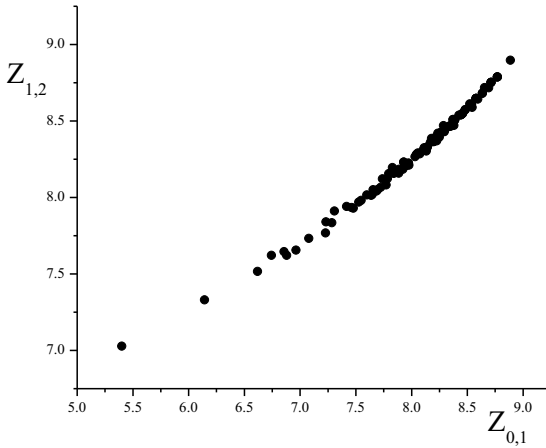
$$Z_{p,q}(G) = \sum_{uv \in E(G)} \frac{M_p(d_u, d_v)}{M_q(d_u, d_v)}.$$

It is evident that  $GA_1(G) \equiv Z_{0,1}$ . In addition, it should be noted that also  $Z_{-1,0}$  coincides with  $GA_1(G)$ , which can be deduced from the well-known equality  $(M_0)^2 = M_1 \cdot M_{-1}$  [20].

We examined correlations between indices  $Z_{p,q}$  for  $-2 \leq p, q \leq 2$  with  $GA_1$  index for several sets of trees. In all studied cases (namely,  $Z_{-2,-1}, Z_{-2,0}, Z_{-2,1}, Z_{-2,2}, Z_{-1,-2}, Z_{-1,1}, Z_{-1,2}, Z_{0,-2}, Z_{0,-1}, Z_{0,2}, Z_{1,-2}, Z_{1,-1}, Z_{1,0}, Z_{1,2}, Z_{2,-2}, Z_{2,-1}, Z_{2,0}, Z_{2,1}$ ), it was found that the  $GA_1$  index is well correlated. Two examples of these correlations are given in Figs. 1 and 2.



**Figure 1.** Correlation between  $Z_{p,q}$  ( $p = -1$ ,  $q = -2$ ) index and first geometric–arithmetic index for 10-vertex trees



**Figure 2.** Correlation between  $Z_{p,q}$  ( $p = 1$ ,  $q = 2$ ) index and first geometric–arithmetic index for 10-vertex trees

The obtained results indicate that the ratio between geometric and arithmetic means in the definition of the first geometric–arithmetic index is not a necessary choice. Other

$Z_{p,q}$  indices may be used in chemical researches instead of it. However, there is no scientific justification for introducing new indices of this kind, because the  $GA_1$  index gathers the same information on observed molecule as other  $Z_{p,q}$  indices.

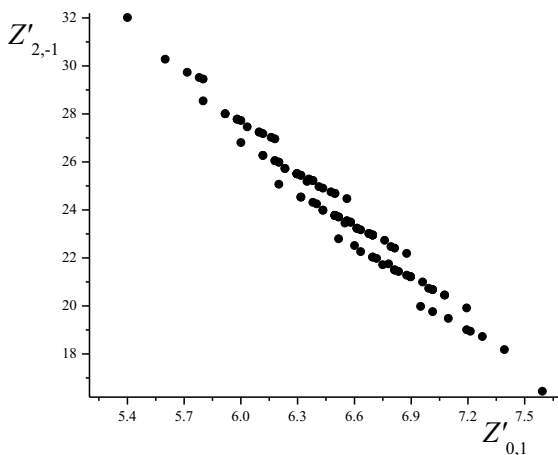
Recently the same “experiment” was made for the second and the third geometric–arithmetic indices. Similarly, as above we defined new classes of indices as follows:

$$Z'_{p,q}(G) = \sum_{uv \in E(G)} \frac{M_p(n_u, n_v)}{M_q(n_u, n_v)} \quad GA_2(G) \equiv Z'_{0,1}$$

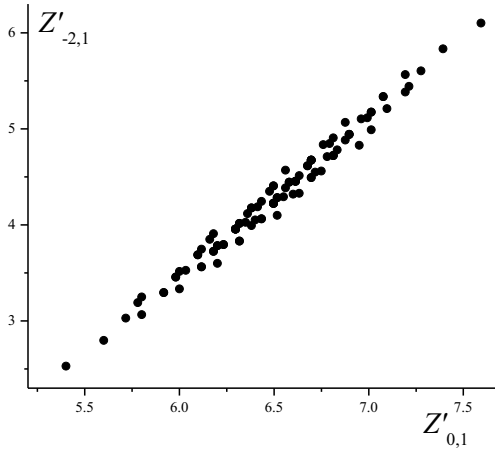
$$Z''_{p,q}(G) = \sum_{uv \in E(G)} \frac{M_p(m_u, m_v)}{M_q(m_u, m_v)} \quad GA_3(G) \equiv Z''_{0,1}$$

where,  $-2 \leq p, q \leq 2$ .

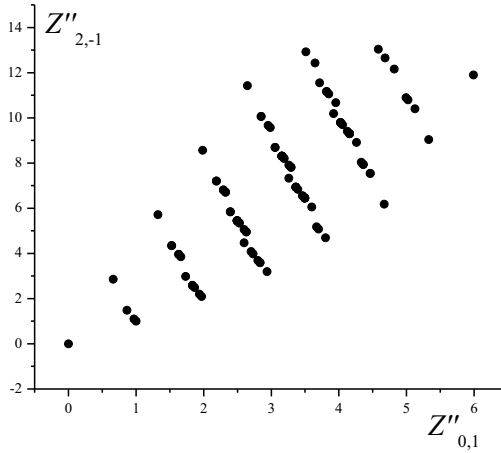
Few examples are shown on Figs. 3–6.



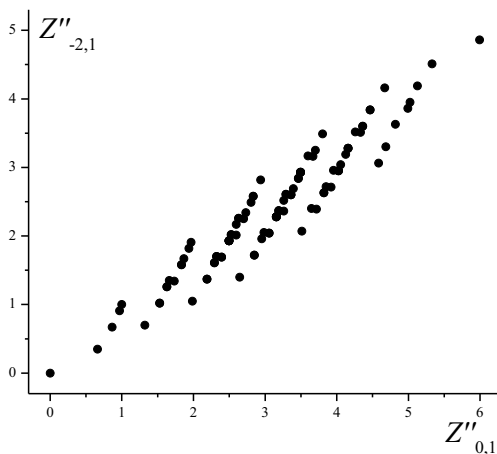
**Figure 3.** Correlation between  $Z'_{p,q}$  ( $p = 2, q = -1$ ) index and second geometric–arithmetic index for 10-vertex trees



**Figure 4.** Correlation between  $Z'_{p,q}$  ( $p = -2$ ,  $q = 1$ ) index and second geometric-arithmetic index for 10-vertex trees



**Figure 5.** Correlation between  $Z''_{p,q}$  ( $p = 2$ ,  $q = -1$ ) index and third geometric-arithmetic index for 10-vertex trees



**Figure 6.** Correlation between  $Z''_{p,q}$  ( $p = -2$ ,  $q = 1$ ) index and third geometric–arithmetic index for 10-vertex trees

From these figures it is seen that there is no straightforward correlation between  $GA_2$  (respectively  $GA_3$ ) index and other  $Z'_{p,q}$  (respectively  $Z''_{p,q}$ ) indices. Nevertheless, by detailed inspection, it was observed that the data-points are clustered into several groups by the number of pendent vertices. The data-points belonging to a group with the same number of pendent vertices are further clumped by the number of subgraphs consisting of two adjacent vertices of degree 1 and 2. These results show that indices  $Z'_{p,q}$  and  $Z''_{p,q}$  carry information on the structure of graphs somewhat different than  $GA_2(G)$  and  $GA_3(G)$  and should be investigated as separate structural descriptors.

### 3. 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 ( $\chi$ ) [79]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (for example see [41, 67, 68] and the references cited therein). During years of research, scientists were trying to improve the predictive power of the

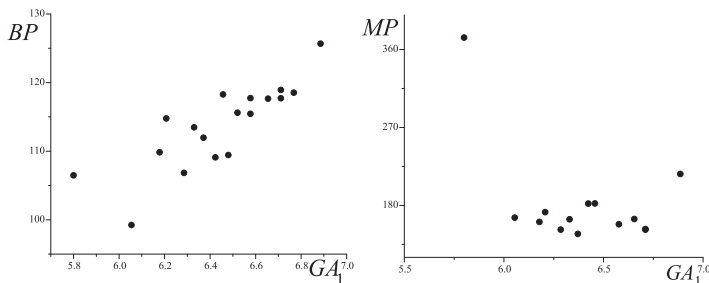


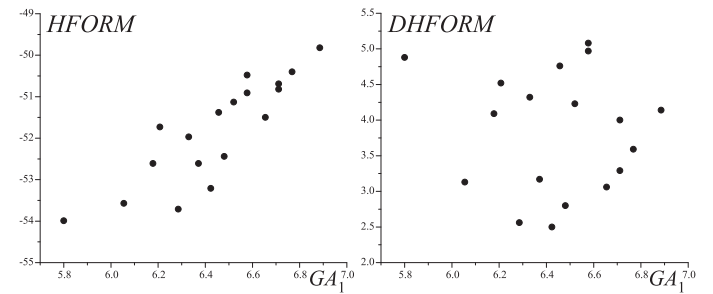
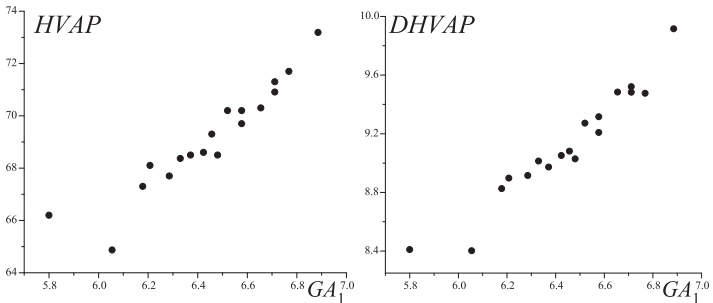
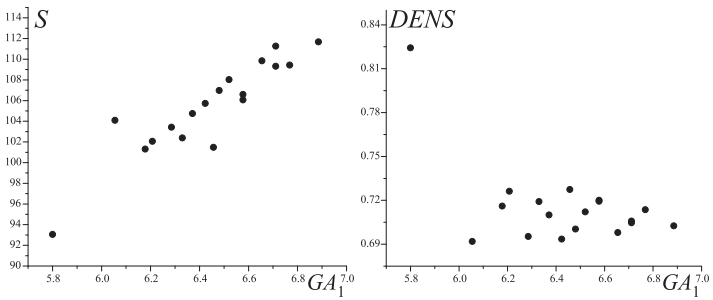
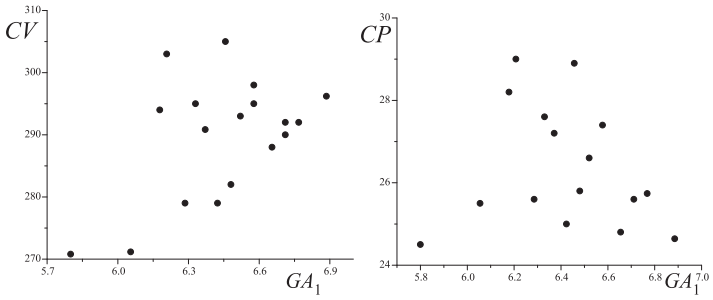
Randić index. This led to the introduction of a number of modifications and new topological descriptors resembling the original  $\chi$ -index. The *first geometric-arithmetic index* ( $GA_1$ ) may be viewed as one of the successors of the Randić connectivity index.

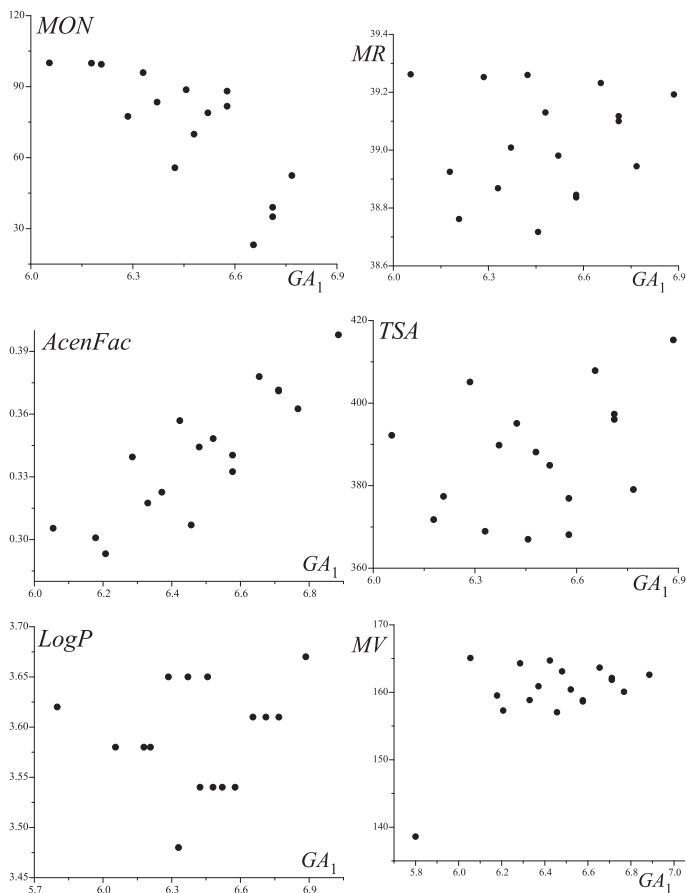
The  $GA_1$  index, defined by Eq. (2), has been introduced less than a year ago [87]. However, a few papers already appeared dealing with this quantity. In the subsequent section, the hitherto obtained results on  $GA_1$  will be summarized.

### 3.1. $GA_1$ 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](http://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 [87] 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	
<i>BP</i>	0.823	0.821	0.562
<i>S</i>	0.912	0.906	2.942
<i>HVAP</i>	0.941	0.936	4.152
<i>DHVAP</i>	0.966	0.958	9.005
<i>HFORM</i>	0.858	0.850	2.494
<i>AcenFac</i>	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  $\chi$ ) 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 [37] and the references cited therein.

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 [85]. 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 [82], is given in Table 2.

<sup>1</sup>The  $RQR$  value can be calculated using the following formula

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

Name	$n$	$\Delta H_f$ (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
naphthacene	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> ]naphthacene	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

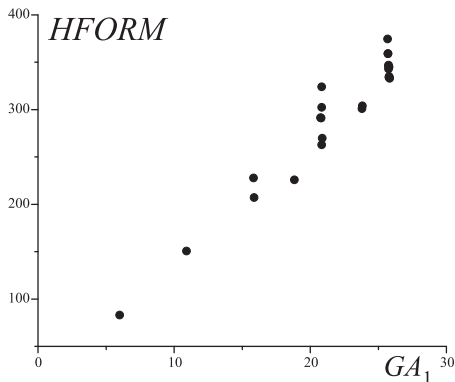
**Table 2.** Heat of formation and the  $GA_1$  index of some benzenoid hydrocarbons

The correlation graphic between the  $GA_1$  indices and heat of formation of the 25 benzenoid hydrocarbons from Table 2 is shown in Fig. 7. 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.

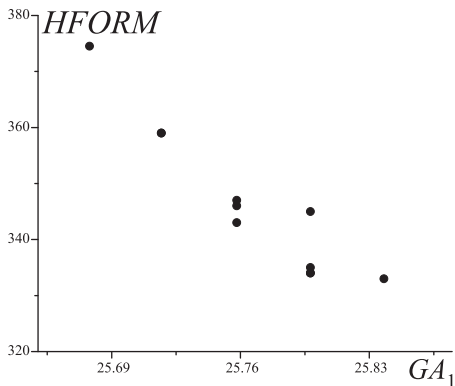
However, it is well known that the heat of formation roughly depends on the number of atoms in the molecule, and therefore the correlation shown in Fig. 7 may, in fact, look unrealistically good. In order to overcome this problem, the examination of correlation between heat of formation and  $GA_1$  index should be limited to isomers. Among experimental results given in Table 1 there are all twelve catacondensed<sup>2</sup> 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

<sup>2</sup>Benzenoid hydrocarbons containing no internal carbon atoms (carbon atoms belonging to three six-membered rings) are said to be "catacondensed".

5 benzene rings is shown in Fig. 8.



**Figure 7.** Heat of formation vs.  $GA_1$  for the 25 benzenoid hydrocarbons from Table 2.



**Figure 8.** Correlation between  $GA_1$  and the heat of formation for all catacondensed benzenoid hydrocarbons with 5 hexagons (i. e., with 22 carbon atoms)

The correlation coefficient is  $-0.939$ . It should be noted from Fig. 8 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.

### 3.2. 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.

#### 3.2.1. 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

$$0 \leq GA_{general}(G) \leq m \leq \binom{n}{2}. \tag{8}$$

The equality on the right–hand side of (8) 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. (8) applied to  $GA_1$  yields the first inequality for that index [87]:

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

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 [87] the following inequality was 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  $(S_n)$ .

The authors of [95] 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 [73] the following lower and upper bounds are reported for  $GA_1$  of a simple  $n$ -vertex graph, with no isolated vertex, and  $m$  edges, in terms of the first Zagreb index  $(M_1)$  and the second Zagreb index  $(M_2)$ :

$$(i) \quad GA_1(G) \geq \frac{2m}{n} \tag{9}$$

$$(ii) \quad GA_1(G) \geq \sqrt{\frac{M_2(G)}{(n-1)^2} + \frac{4m(m-1)}{n^2}} \tag{10}$$

$$(iii) \quad GA_1(G) \leq \frac{1}{2}M_1(G) \tag{11}$$

with equality if and only if  $G$  is a union of  $K_2$ ;

$$(iv) \quad GA_1(G) \leq \sqrt{mM_2(G)} \tag{12}$$

with equality if and only if  $G$  is a union of  $K_2$ ;

$$(v) \quad GA_1(G) \leq \sqrt{M_2(G) + m(m-1)} \tag{13}$$

with equality if and only if  $G$  is a union of  $K_2$ ;

$$(vi) \quad GA_1(G) \leq \left\lceil \frac{m-1}{2} \right\rceil + \sqrt{\left\lceil \frac{m-1}{2} \right\rceil^2 + M_2(G)} \tag{14}$$

with equality if and only if  $G$  is a union of an odd number of  $K_2$ .

In [11] a lower bound for  $GA_1$  of a simple graph  $G$  with  $m$  edges, in terms of maximum vertex degree ( $\Delta$ ) and minimum vertex degree ( $\delta$ ) 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 [11] a lower and an upper bound for  $GA_1$  was reported in following terms:

$\delta_1$  – minimum non-pendent vertex degree

$d_1, d_2, \dots, d_n$  – degree sequence

$M_2(G)$  – second Zagreb index

$\nu$  – number of pendent vertices

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

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

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

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



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

In [13] a lower bound for  $GA_1$  of a simple connected graph with  $m$  edges, in terms of maximum degree  $(\Delta)$ , minimum non-pendent vertex degree  $(\delta_1)$  and number of pendent vertices  $(\nu)$  was presented.

$$GA_1(G) \geq \frac{2\nu\sqrt{\Delta}}{\Delta+1} + \frac{1}{\Delta} \sqrt{M_2(G) - \nu\Delta + (m-\nu)(m-\nu-1)\delta_1^2}$$

with equality if and only if  $G \cong K_{1,m-1}$  or  $G$  is isomorphic to regular graph or  $G$  is isomorphic to  $(\Delta, 1)$ -semiregular graph.

In the same paper another lower bound for all connected graphs with  $m$  edges it was given, in terms of maximum degree  $(\Delta)$ , minimum non-pendent vertex degree  $(\delta_1)$ , number of pendent vertices  $(\nu)$  and degree sequence  $d_1, d_2, \dots, d_n$

$$GA(G) \geq \frac{2\nu\sqrt{\Delta}}{\Delta+1} + \frac{\sqrt{8(\Delta+\delta_1)\sqrt{\Delta}\delta_1}}{(\sqrt{\Delta}+\sqrt{\delta_1})^2} \sqrt{(m-\nu)^2 - \frac{m-\nu}{4\delta_1^2} \left( \sum_{i=1}^n d_i^3 - 2M_2(G) - \nu(\delta_1-1)^2 \right)}$$

where  $M_2(G)$  is the second Zagreb index of  $G$ . Moreover, the equality holds if and only if  $G$  is isomorphic to a regular graph or  $G$  is isomorphic to a  $(\Delta, 1)$ -semiregular graph.

A further lower bound on  $GA_1$  is [13]:

$$GA_1(G) \geq \frac{2m\sqrt{2(n-1)}}{n+1} - 2\nu \left( \frac{\sqrt{2(n-1)}}{n+1} - \frac{\sqrt{n-1}}{n} \right) \tag{15}$$

with equality if and only if  $G$  is isomorphic to the star  $K_{1,n-1}$  or  $G$  is isomorphic to the complete graph  $K_3$ .

An analogous upper bound on  $GA_1$  for connected graphs with  $m$  edges, in terms of second Zagreb index  $(M_2)$  and minimum degree  $(\delta)$  is [13]:

$$GA_1(G) \leq \frac{\sqrt{mM_2(G)}}{\delta} \tag{16}$$

with equality if and only if  $G$  is isomorphic to a regular graph. Moreover [13],

$$\frac{1}{\Delta} \sqrt{M_2(G) + m(m-1)\delta^2} \leq GA_1(G) \leq \frac{1}{\delta} \sqrt{M_2(G) + m(m-1)\Delta^2} \tag{17}$$

with equality on the both sides if and only if  $G$  is isomorphic to regular graph. For all connected graphs the lower and upper bounds in (17) are better than (10) and (13), respectively.

Nordhaus–Gaddum type [76] lower and upper bounds for a connected graph  $G$  and its connected complement graph  $\overline{G}$  were obtained in [11]:

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

where  $k = \max \left\{ \sqrt{\frac{\Delta}{\delta}}, \sqrt{\frac{n-1-\delta}{n-1-\Delta}} \right\}$ .  $\nu$ ,  $\overline{\nu}$ , and  $\delta_1$ ,  $\overline{\delta_1}$  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.

The Cartesian product  $G_1 \times G_2$  of graphs  $G_1$  and  $G_2$  is a graph such that  $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ , and any two vertices  $(a, b)$  and  $(u, v)$  are adjacent in  $G_1 \times G_2$  if and only if either  $a = u$  and  $b$  is adjacent with  $v$ , or  $b = v$  and  $a$  is adjacent to  $u$ . In [73] the  $GA_1$  indices for  $P_k \times P_l$  and  $C_k \times P_l$  were found to be the following:

$$GA_1(P_k \times P_l) = 2kl - 3(k+l) + 8(k+l-4) \frac{\sqrt{3}}{7} + \frac{16\sqrt{6}}{5}$$

and

$$GA_1(C_k \times P_l) = 2k(l-1) + \frac{8k\sqrt{3}}{7}.$$

### 3.2.1.1. 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* [83].

In [95] 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 vertices of degree four and one. The right equality is reached if and only if  $G$  is a path or a cycle.

**3.2.2. 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 [87] explored mathematical properties of  $GA_1$  of trees and chemical trees. They obtained the following tight lower and upper bounds for trees:

$$\frac{2(n-1)^{3/2}}{n} = GA_1(S_n) \leq GA_1(T) \leq GA_1(P_n) = \begin{cases} 0 & n = 1 \\ 1 & n = 2 \\ \frac{4\sqrt{2}}{3} + n - 3 & n \geq 3 \end{cases} \quad (18)$$

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 ( $P_n$ ).

**3.2.2.1. 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 (18). The lower bound for chemical trees is given in [87]:

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

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.

$n$	$\eta$
5	1
8	1
11	1
14	2
17	3
20	5

**Table 3** Among chemical trees with  $n$  vertices there are  $\eta$  trees having minimal  $GA_1$  index.

In [95] 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 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  $\frac{13}{15}n + \frac{8\sqrt{2}}{3} + \frac{12\sqrt{3}}{7} - \frac{39}{5}$ .

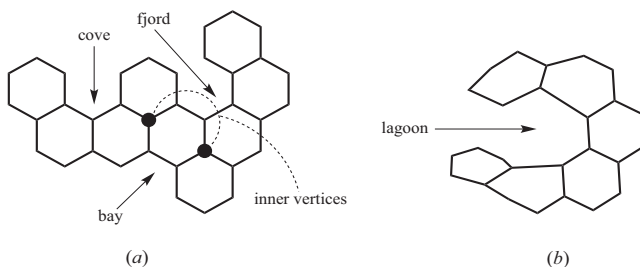
In addition, the same authors determined the chemical trees with second and third maximal  $GA_1$  index.

- (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  $n - 6 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$ .

Recently, a paper appeared considering among others the  $GA_1$  index of eight classes of graphs. [21]

### 3.2.3. $GA_1$ 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. 9 (a). Hexahelicene (Fig. 9 (b)) does not belong to the class of benzenoid hydrocarbons because it does not obey the condition of planarity.



**Figure 9.** (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.

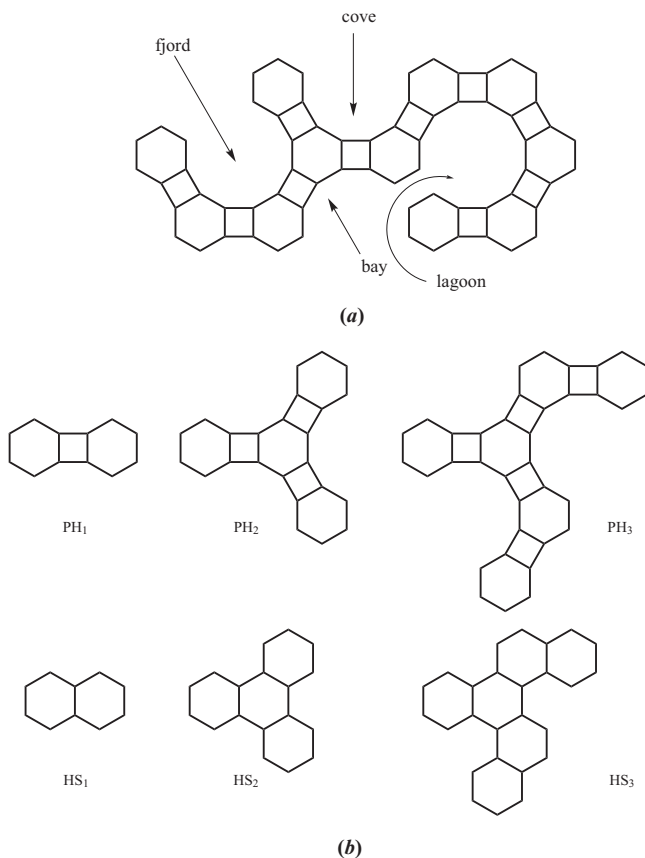
Phenylenes are a class of alternant polycyclic conjugated molecules consisting of six- and four-membered rings, so that each four-membered ring is adjacent to two (disjoint) six-membered rings, and no two six-membered rings are adjacent. K. P. C. Vollhardt with his group synthesized a large number of phenylenes (for details see [88,89]). They attracted much attention of theoretical chemists because of their specific structure (containing both stabilizing six-membered, and destabilizing four-membered rings) [4,40,84]. Structural features such as bays, coves, fjords, and lagoons can be found also in the structural formulas of phenylenes (see Fig. 10(a)). Phenylenes do not have internal 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 whose topology corresponds to the considered phenylene) [26,27,29,32,34,38,40,45,47,48,77,78]. 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. 10(b).

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 [9,37].

Thus,

$$\begin{aligned}
 n_i &= \text{number of internal vertices} \\
 h &= \text{number of hexagons} \\
 B &= \text{number of bays} \\
 C &= \text{number of coves} \\
 F &= \text{number of fjords} \\
 L &= \text{number of lagoons} \\
 b &= \text{number of bay regions; } b = B + 2C + 3F + 4L
 \end{aligned}$$



**Figure 10.** (a) Phenylenes possess all structural properties noticed already in benzenoid hydrocarbons (cf. Fig. 9), except internal vertices. (b) Phenylenes  $PH_1$ ,  $PH_2$ ,  $PH_3$  and the corresponding hexagonal squeezes  $HS_1$ ,  $HS_2$ ,  $HS_3$ .

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

$$GA_1(B) = \frac{8\sqrt{6} + 5}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{4\sqrt{6} - 5}{5}n_i - \frac{8\sqrt{6} - 25}{5}. \quad (19)$$

For catacondensed benzenoid hydrocarbons (i. e., hexagonal squeezes) Eq. (19) is reduced by deleting the term  $\frac{4\sqrt{6}-5}{5}n_i$ :

$$GA_1(HS) = \frac{8\sqrt{6} + 5}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{8\sqrt{6} - 25}{5}. \quad (20)$$

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

$$GA_1(PH) = \frac{8\sqrt{6} + 20}{5}h - \frac{4\sqrt{6} - 10}{5}b - \frac{8\sqrt{6} - 10}{5}. \quad (21)$$

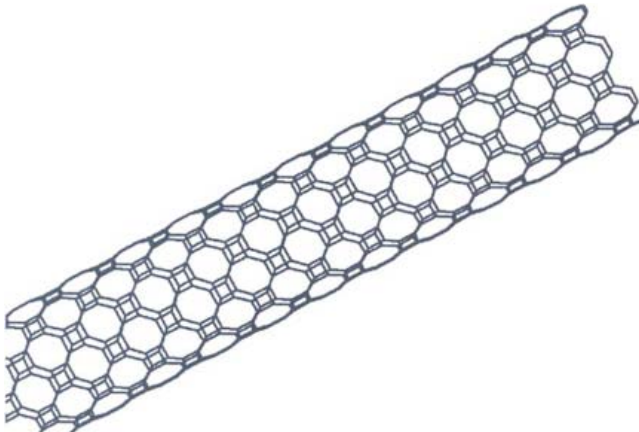
Combining Eqs. (20) and (21) we get linear relation between  $GA_1$  of phenylene and its hexagonal squeeze [91]:

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

### 3.2.4. $GA_1$ index of nanostructures

Since the discovery of buckminsterfullerene [65] and latter of nanotubes [57], 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 examined many structures of fullerenes, nanotubes, nanotoruses, . . . , expecting to be synthesized in the future [19].

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 [1, 2, 51, 52, 58, 59, 92]. In Fig. 11 is shown the structure of this type of nanotubes.

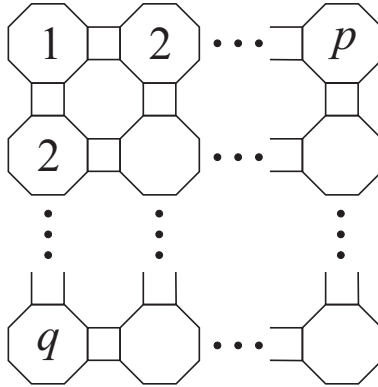


**Figure 11.** A  $TUC_4C_8(S)$  nanotube

In [30] exact formulas for the 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 ( $HTUC[p, q]$ ) are found, in terms of the parameters  $p$  and  $q$ . The two-dimensional lattice of the  $TUC_4C_8(S)$  graph is tessellated by alternating squares ( $C_4$ ) and octagons ( $C_8$ ) as it is shown in Fig. 12.



**Figure 12.** 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

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

The results on  $GA_1$  index of nanostructures are continuously growing. For example see [7, 54].

## 4. 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 [24]. It is also based on Eq. (1), and its definition is given by Eq. (5).

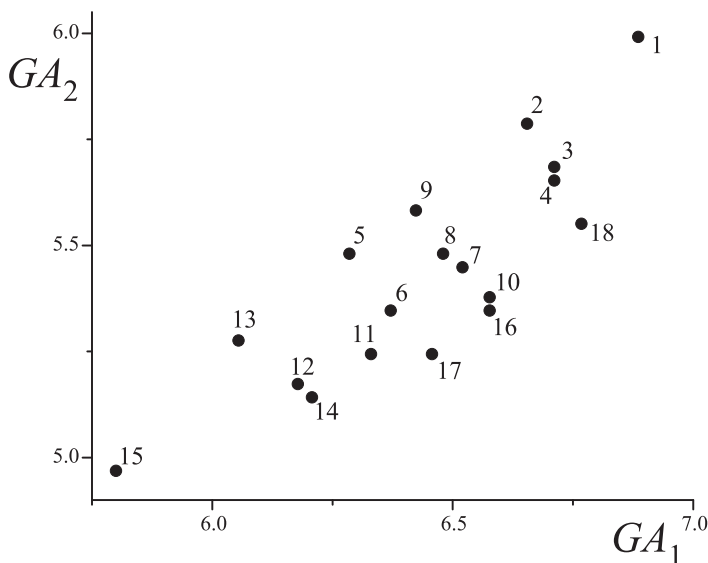
### 4.1. $GA_2$ as a tool for QSAR/QSPR researches

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. 13 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



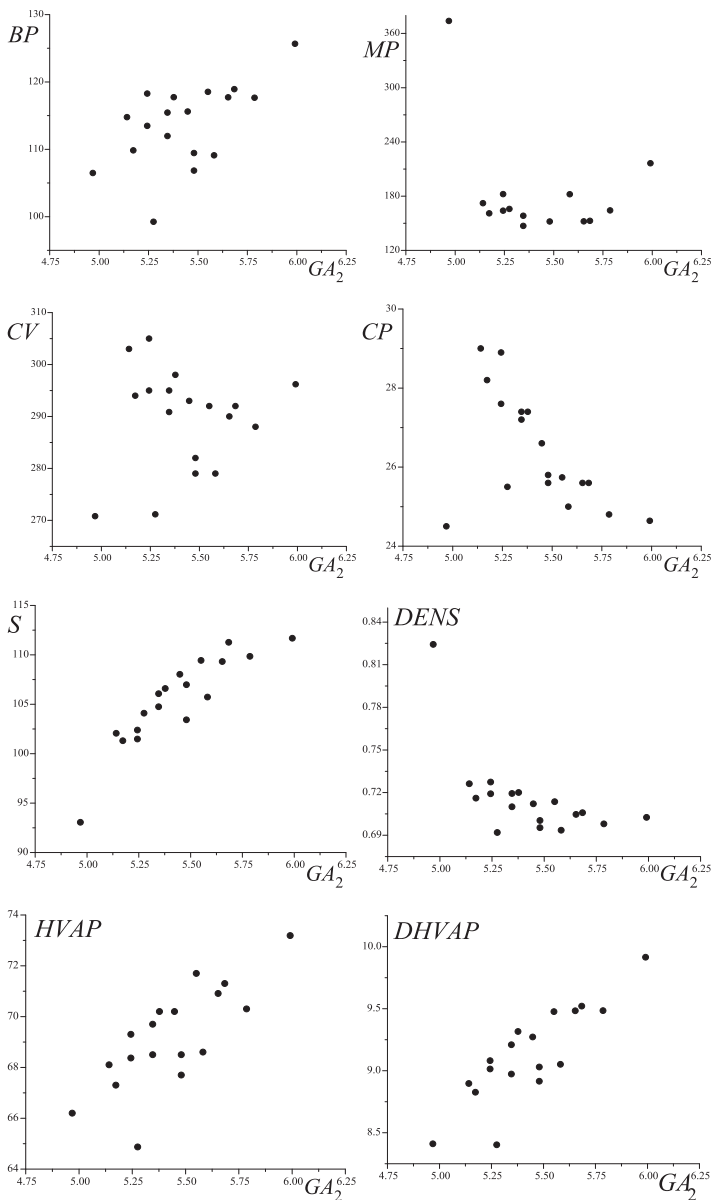
**Figure 13.** Correlations between  $GA_1$  and  $GA_2$  of octanes; the numbering of the data points corresponds to Table 4.

A detailed examination of Fig. 13 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  $(n_4, n_3) = (0, 3)$ .

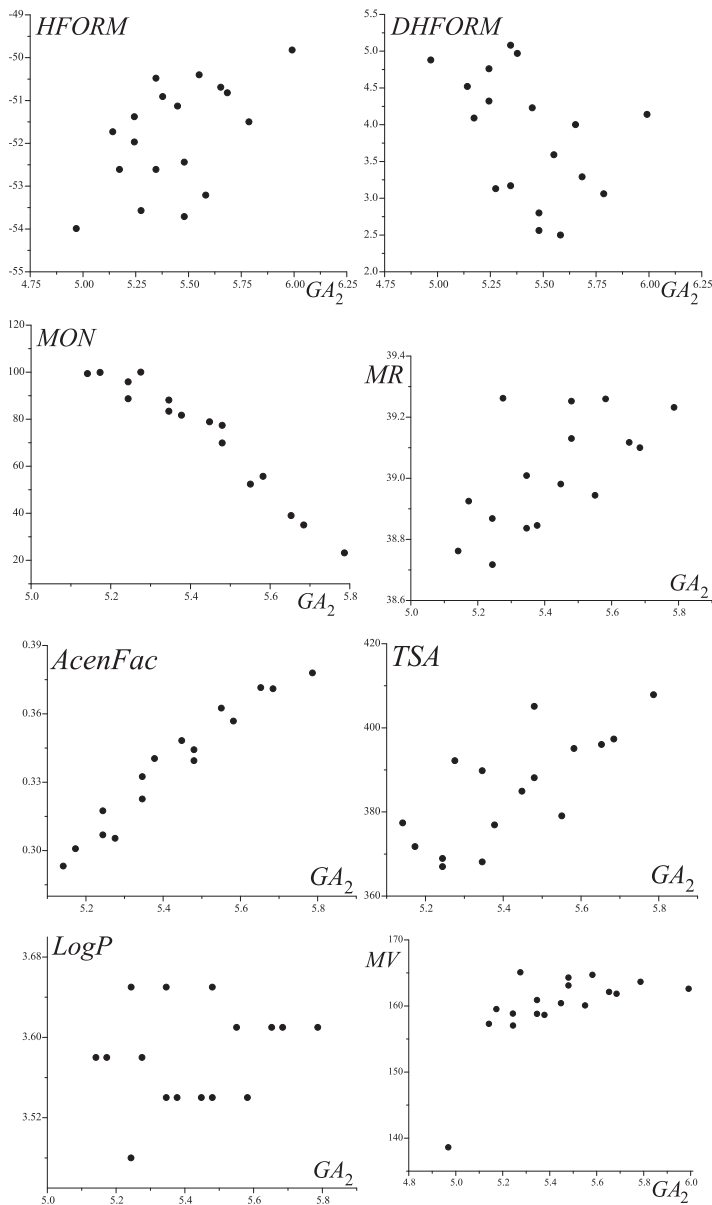
Thus, the isomers belonging to the same cluster are those similarly branched. Within each such cluster (provided that there are two or more data points), the proportionality between  $GA_1$  and  $GA_2$  is inverse. For instance, the data points **7**, **8**, **9**, **10**, and **16**, all pertaining 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 ( $DHVAP$ ), 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
$DHVAP$	0.843
$MON$	0.968
$AcenFac$	0.973

Table 5.

## 4.2. Mathematical properties of $GA_2$

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

### 4.2.1. Lower and upper bounds for $GA_2$

Lower and upper bounds of  $GA_2$  index for bipartite graphs were communicated in [24, 96]:

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

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 [24]:

$$GA_2(G) \geq \frac{2m\sqrt{n-1}}{n}. \tag{22}$$

Equality in (22) 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 ( $PI_v$ ) [62] has been introduced recently inspired by the definition of the “original”  $PI$  index which already had many applications in chemistry (e.g. see [18] 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 [61, 71, 74, 75].

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 [33]:

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

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 [39]. Chemical applications of the Szeged index were presented in the book [18].

For all connected graphs the following inequality is true [24]:

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

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

$$GA_2(G) \leq \sqrt{m Sz(G)} \tag{23}$$

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

In [96] 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 [24] it was proven that for all connected graphs:

$$GA_2(G) \leq \sqrt{Sz(G) + m(m-1)} \tag{24}$$

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

For the complete graph, the inequalities (23) and (24) are equivalent. For all other connected graphs, the upper bound (24) is better than (23).

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:

$$GA_2(G) \geq \frac{2}{n} \sqrt{Sz(G) + m(m-1)}. \tag{25}$$

Equality in (25) is attained if and only if  $G \cong K_2$ .

For the complete graph with two vertices, inequalities (25) and (22) are equivalent. For all other connected graphs the lower bound (22) is better than (25).

In addition, in [24] it was also proven that the star  $K_{1,n-1}$  is the connected  $n$ -vertex graph with minimum second geometric–arithmetic index.

In [14] a lower bound for  $GA_2$  of a simple graph  $G$  on  $n$  vertices with  $m$  edges and number of pendent vertices  $\nu$  was presented:

$$GA_2(G) \geq \frac{2m\sqrt{n-2}}{n-1} - 2\nu \left( \frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n} \right). \tag{26}$$

Equality holds if and only if  $G$  is isomorphic to the star  $K_{1,n-1}$  or  $G$  is isomorphic to the complete graph  $K_3$ .

For all connected graphs the lower bound (26) is better than the lower bounds (22) and (25).

Let  $\Gamma_1$  be the class of graphs  $H_1 = (V_1, E_1)$  such that  $H_1$  is connected with  $n_i = n_j$  for each edge  $ij \in E(H_1)$ . For example,  $K_{1,n-1}, K_n \in \Gamma_1$ . Denote by  $C_n^*$  a unicyclic graph of order  $n$  and cycle length  $k$  such that each vertex in the cycle is adjacent to one pendent vertex,  $n = 2k$ . Let  $\Gamma_2$  be the class of graphs  $H_2 = (V_2, E_2)$  such that  $H_2$  is connected with  $n_i = n_j$  for each non-pendent edge  $ij \in E(H_2)$ . For example,  $C_n^* \in \Gamma_2$ :

In [14] an upper bound on  $GA_2$  index of simple connected graph  $G$  of order  $n$  with  $m$  edges and  $\nu$  pendent vertices was obtained:

$$GA_2(G) \leq \frac{2\nu\sqrt{n-1}}{n} + m - \nu. \tag{27}$$

Equality holds if and only if  $G \cong K_{1,n-1}$  or  $G \in \Gamma_1$  or  $G \in \Gamma_2$ .

For all connected graphs the upper bound (27) is better than the upper bounds (23) and (24).

Nordhaus–Gaddum-type [76] lower and upper bounds for a connected graph  $G$  and its connected complement  $\overline{G}$  were obtained in [14].



$$\begin{aligned} & \frac{2\sqrt{n-2}}{n-1} \binom{n}{2} - 2(\nu + \bar{\nu}) \left( \frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n} \right) \\ & < GA_2(G) + GA_2(\bar{G}) \leq \\ & \binom{n}{2} - (\nu + \bar{\nu}) \left( 1 - \frac{2\sqrt{n-1}}{n} \right), \end{aligned} \tag{28}$$

where  $n$  is the number of vertices,  $\nu$  and  $\bar{\nu}$  are the number of pendent vertices in  $G$  and  $\bar{G}$ , respectively.

**4.2.2. Extremal values of the  $GA_2$  index of trees**

The trees with extremal values of  $GA_2$  index are presented in the paper [24]. 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  $GA_2$ .

A tree is said to be starlike if exactly one of its vertices has degree greater than two. By  $S(2r, s)$  ( $r \geq 1, s \geq 1$ ), we denote the starlike tree with diameter less than or equal to 4, which has a vertex  $v_1$  of degree  $r + s$  and which has the property  $S(2r, s) \setminus \{v_1\} = \underbrace{P_2 \cup P_2 \cup \dots \cup P_2}_r \cup \underbrace{P_1 \cup P_1 \cup P_1}_s$ . This tree has  $2r + s + 1 = n$  vertices. We say that the starlike tree  $S(2r, s)$  has  $r + s$  branches, the lengths of which are  $\underbrace{2, 2, \dots, 2}_r, \underbrace{1, 1, \dots, 1}_s$ , respectively. For  $p, q \geq 2$ , let  $S_{p,q}$  be the  $(p + q)$ -vertex tree, formed by adding an edge between the centers of the stars  $K_{1,p-1}$  and  $K_{1,q-1}$ .

In [14] a lower bound for  $GA_2$  of a tree  $T$  on  $n$  vertices with  $\nu$  pendent vertices was presented:

$$GA_2(T) \geq \frac{2m\sqrt{2(n-2)}}{n} - \frac{2\nu}{n} \left( \sqrt{2(n-2)} - \sqrt{n-1} \right).$$

Equality holds if and only if  $T \cong K_{1,n-1}$  or  $T \cong S(2r, s), n = 2r + s + 1$ .

In the same paper an upper bound for  $GA_2$  was obtained:

$$GA_2(T) \leq n - 1 - \nu + \frac{2\nu\sqrt{n-1}}{n}$$

with equality if and only if  $T \cong K_{1,n-1}$  or  $T \cong S_{q,q}$ ,  $n = 2q$ .

Let  $P_{d+1}(i, n-d-1)$  denote the tree in  $T_{n,d}$  obtained from the path  $P_{d+1} = v_1 \cdots v_{d+1}$  by attaching to its  $i$ th vertex ( $2 \leq i \leq d$ )  $n-d-1$  leaves. Denote by  $T_{n,d}$ , the set of trees with  $n$  vertices and diameter  $d$ .

In [55] it has been shown that among all trees in  $T_{n,d}$ , the tree  $P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$  has the minimum  $GA_2$  index. More on the mathematical properties of  $GA_2$  index can be found in [56, 80].

## 5. 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 [96] and is defined by Eq. (6). Some of its properties are discussed in this section.

### 5.1. $GA_3$ 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. 14 and 15 show these correlations.

Comparing Figs. 13 and 14 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. 14 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. 15.

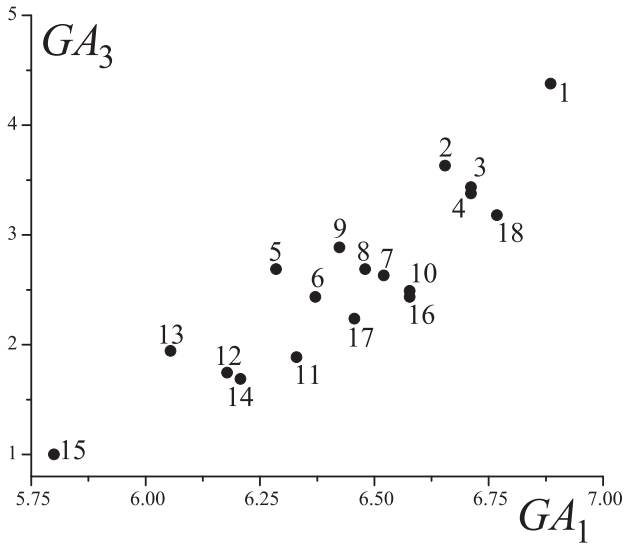


Figure 14.

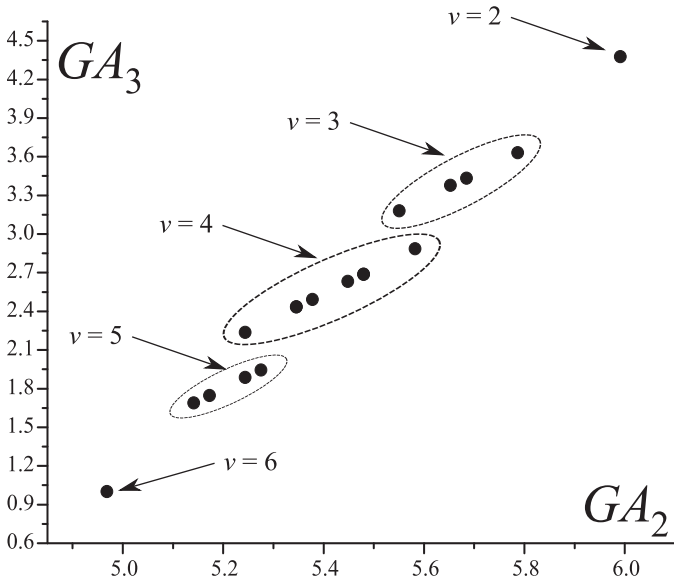


Figure 15.

By a superficial glance at Fig. 15 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 ( $\nu$ ) in a 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.

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

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

**Table 6.**  $\nu$  is the number of pendent vertices;  $a$  and  $\Delta a$  are the slope of the line and the respective absolute error;  $b$  and  $\Delta b$  are the intercept of the line and the respective absolute error;  $R$  is the correlation coefficient.

From the results presented in Table 6, it is evident that there exists a correlation between  $GA_3$  and  $GA_2$  in the following sense:

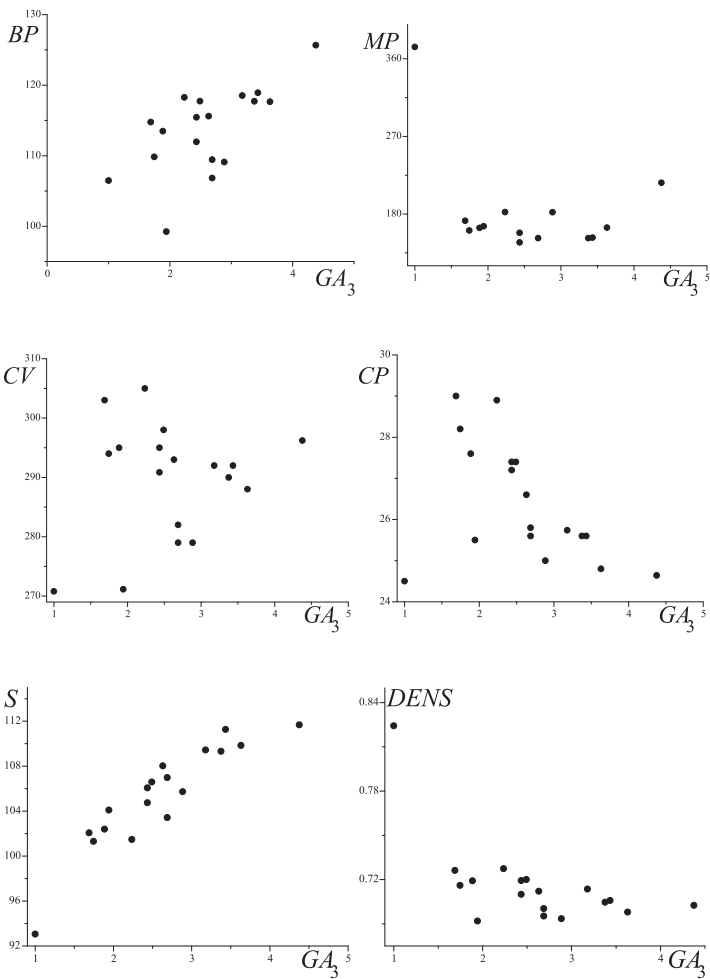
$$GA_3(T) = \alpha * GA_2(T) + \beta * \nu + \gamma \tag{29}$$

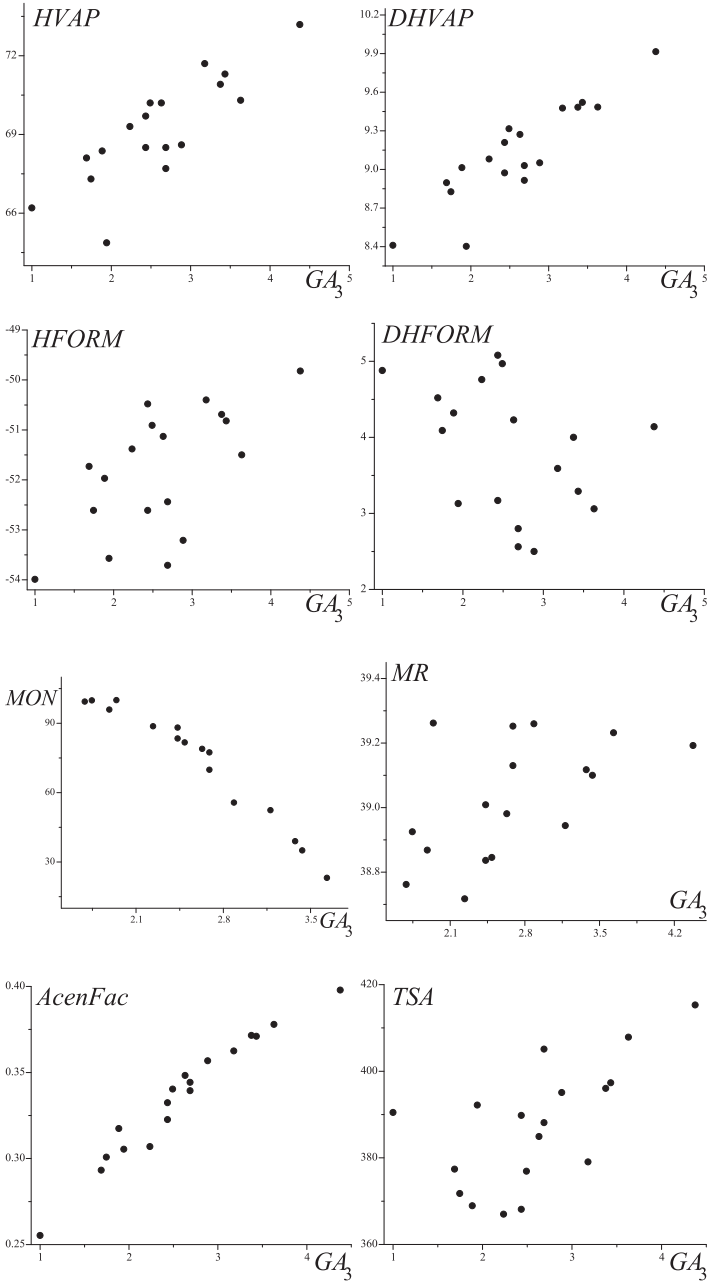
We succeeded to mathematically explain this peculiar correlation between  $GA_2$  and  $GA_3$  indices by showing that  $GA_3$  is bounded from both below and above by an expression that is an increasing function of  $GA_2$  and a decreasing function of  $\nu$  [28, 44].

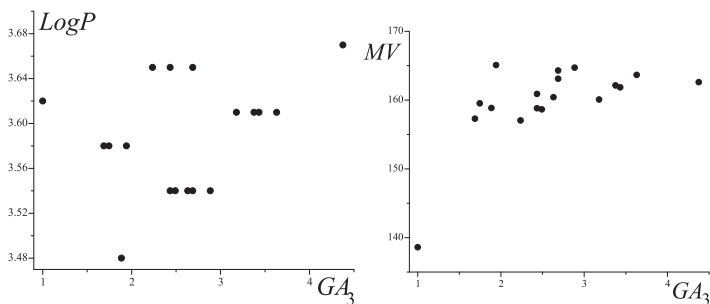
$$\frac{n}{n-2} GA_2(T) - \frac{2\sqrt{2(n-1)(n-2)} - 2(n-1)}{(n-2)\sqrt{2(n-2)}} \nu - \frac{2(n-1)^2}{(n-2)\sqrt{2(n-2)}} < GA_3(T) < \frac{n}{n-2} GA_2(T) - \frac{2\sqrt{(n-1)\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor} - n + 1}{(n-2)\sqrt{\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor}} \nu - \frac{(n-1)^2}{(n-2)\sqrt{\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor}} \tag{30}$$

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 correlations ( $R \geq 0.8$ ) 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  $GA_2$ .

## 5.2. 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. 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 [36]

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

For more results about the edge-Szeged index consult the papers [3, 6, 8, 63, 64, 86].

**5.2.1. Lower and upper bounds for  $GA_3$**

For all connected graphs with  $n$  vertices the following inequality holds [96]:

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

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:

$$\frac{2}{m-1} \sqrt{Sz_e(G)} \leq GA_3(G) \leq \sqrt{Sz_e(G) + m(m-1)} . \tag{31}$$

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

In [15] it another lower bound for  $GA_3$  was obtained, for connected graphs with  $m$  edges and  $\nu$  pendent vertices:

$$GA_3(G) \geq \frac{2(m-\nu)\sqrt{m-2}}{m-1} \tag{32}$$

with equality if and only if  $G \cong K_{1,n-1}$  or  $G \cong K_3$  or  $G \cong S(2r, s)$ ,  $n = 2r + s + 1$ .

Also in [15] another lower bound was deduced,

$$GA_3(G) \geq \frac{2}{m-1} \sqrt{Sz_e(G) + (m-\nu)(m-\nu-1)(\delta_1-1)^2} \tag{33}$$

where  $Sz_e(G)$  and  $\delta_1$  are the edge-Szeged index and minimum non-pendent vertex degree in  $G$ , respectively. Equality holds if and only if  $G \cong K_{1,m}$  or  $G \cong K_3$  or  $G \cong S_{\nu,m+1-\nu}$ ,  $2 \leq \nu \leq [(m+1)/2]$ .

For all connected graphs the lower bound (33) is better than the lower bound (31).

Let  $\Gamma_3$  be the class of graphs  $H_3 = (V_3, E_3)$  such that  $H_3$  is connected with  $m_i = m_j$  for each edge  $ij \in E(H_3)$ . For example,  $K_n, C_n \in \Gamma_3$ . Let  $\Gamma_4$  be the class of graphs  $H_4 = (V_4, E_4)$  such that  $H_4$  is connected with  $m_i = m_j$  for each non-pendent edge  $ij \in E(H_4)$ . For example,  $C_n^* \in \Gamma_4$ . Now we are ready to give an upper bound on  $GA_3(G)$  of graph  $G$ .



In [15] an upper bound for  $GA_3$  was obtained:

$$GA_3(G) \leq m - \nu \tag{34}$$

with equality if and only if  $G \cong K_{1,m}$  or  $G \in \Gamma_3$  or  $G \in \Gamma_4$ .

For all connected graphs the upper bound (34) is better than (31).

Nordhaus–Gaddum-type [76] lower and upper bounds for a connected graph  $G$  and its connected complement  $\overline{G}$  were obtained in [15].

$$\frac{2(m - \nu)\sqrt{m - 2}}{m - 1} + \frac{2(\overline{m} - \overline{\nu})\sqrt{\overline{m} - 2}}{\overline{m} - 1} \leq GA_3(G) + GA_3(\overline{G}) \leq \binom{n}{2} - (\nu + \overline{\nu}) \tag{35}$$

where  $n$  is the number of vertices, and  $\nu, \overline{\nu}$ , and  $m, \overline{m}$  are the number of pendent vertices and edges in  $G$  and  $\overline{G}$ , respectively.

### 5.2.2. Extremal values of the $GA_3$ index of trees

In [96] 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  $\Delta$ , where  $2 \leq \Delta \leq n-1$ . Then

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

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

### 5.2.3. Relation between $GA_3$ and $GA_2$ indices of unicyclic graphs

In [28] the relation (30) between the  $GA_2$ - and  $GA_3$ -indices of a tree  $T (\not\cong K_{1,n-1})$  on  $n$  vertices with  $\nu$  pendent vertices ( $2 \leq \nu \leq n-2$ ) was obtained. In this section we present the analogous result for unicyclic graphs.

For unicyclic graphs with girth  $g$ , let  $c_1, c_2, \dots, c_g$  be the vertices belonging to the cycle  $C$ , that is,  $V(C) = \{c_1, c_2, \dots, c_g\}$ . Let  $s$  be the number of vertices of one of maximal components of  $G - V(C)$ . In [70] the following relation between  $GA_2$  and  $GA_3$  of a unicyclic graph  $G$  with even girth and  $\nu$  pendent vertices was obtained. If  $s \leq n/2$ , then

$$\begin{aligned} & \frac{n}{n-1} \left( 1 - \frac{n-1}{2(n-2)} \right) GA_2(G) - \frac{2\nu}{\sqrt{n-1}} \left( 1 - \frac{n-1}{2(n-2)} \right) \\ < GA_3(G) < \frac{n}{n-2} \left( 1 - \frac{n-1}{2 \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil} \right) GA_2(G) - \frac{2\sqrt{n-1}}{n-2} \left( 1 - \frac{n-1}{2 \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil} \right) \nu \end{aligned}$$

and

$$\begin{aligned} & \frac{n}{n-1}GA_2(G) - \left( \frac{2}{\sqrt{n-1}} - \frac{\sqrt{2}}{\sqrt{n-2}} \right) \nu - \frac{\sqrt{2}n}{\sqrt{n-2}} < GA_3(G) \\ < \frac{n}{n-2}GA_2(G) - \left( \frac{2\sqrt{n-1}}{n-2} - \frac{n-1}{(n-2)\sqrt{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}} \right) \nu - \frac{(n-1)n}{(n-2)\sqrt{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}}. \end{aligned}$$

In the same paper [70] also the following relations and given:

$$\begin{aligned} & \frac{n}{n-1} \left[ 1 - \frac{n-1}{2(n-2)} \right] GA_2(G) - \frac{2\nu}{\sqrt{n-1}} \left[ 1 - \frac{n-1}{2(n-2)} \right] \\ < GA_3(G) < GA_2(G) - \frac{2\nu\sqrt{n-1}}{n} + \frac{(3n-8)(n-6)}{4} \end{aligned}$$

and

$$\begin{aligned} & GA_2(G) - (n-g-\nu)\sqrt{n-2} - \frac{2\nu\sqrt{n-1}}{n} \\ < GA_3(G) < GA_2(G) - \frac{(n-g-\nu)}{n(n-1)}\sqrt{2(n-2)} - \frac{2\nu\sqrt{n-1}}{n}. \end{aligned}$$

provided the girth  $g$  girth of  $G$  is odd.

### 5.2.4. Comparing the geometric–arithmetic indices

In [17] the geometric–arithmetic indices were compared for different types of graphs.

(i) For a chemical tree  $T$  of order  $n$ ,

$$GA_1(T) \geq GA_2(T)$$

with equality if and only if  $G$  is isomorphic to the star  $K_{1,i}$ ,  $i = 1, 2, 3, 4$ .

(ii) For a starlike tree  $S(r_1, r_2, \dots, r_k)$  ( $r_1 + r_2 + \dots + r_k + 1 = n$ ) of order  $n$ ,

$$GA_1(S) \geq GA_2(S)$$

with equality if and only if  $S$  is isomorphic to star the  $K_{1,n-1}$ .

(iii) For any tree  $T$ ,

$$GA_2(T) > GA_3(T).$$

In [16] the first geometric–arithmetic index and the  $ABC$ -index (see [25]) were compared for different types of graphs. Denote by  $K_{1,4}$  the star on 5 vertices. Also denote

by  $T^*$  the tree on 8 vertices, obtained by joining the central vertices of two stars  $K_{1,3}$  by an edge.

(i) For a chemical tree  $T$  of order  $n$ ,

$$GA(T) > ABC(T) \quad T \not\cong K_{1,4}, T^*.$$

(ii) For a molecular graph  $G$  of order  $n$ ,

$$GA(G) > ABC(G) \quad G \not\cong K_{1,4}, T^*.$$

(iii) Let  $G$  be a simple graph with maximum degree  $\Delta$  and minimum degree  $\delta$ . If  $\Delta - \delta \leq 3$  and  $G \not\cong K_{1,4}, T^*$ , then

$$GA(G) > ABC(G).$$

## 6. Conclusion

In this survey, probably all results on  $GA$  indices known around the middle of 2010 have been 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 will find reasonable applications in QSAR/QSPR researches.

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