Int. J. Math. And Appl., 6(1)(2018), 155–163. (Special Issue)
ISSN: 2347-1557
Available Online: http://ijmaa.in/

International Journal of *Mathematics And its Applications*

On Multiplicative Geometric Arithmetic Index of Some Chemical Structures

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Abstract: Graph theoretical study of chemical structures is widely used in physico-chemical characterization of molecules. Several numerical quantities known as topological indices that are associated with the graph structures of molecules have been used as a tool for the characterization of chemical structures. Mathematically, a topological index is a function from any structural property of the graph to a positive real number. With many new developments in chemistry, topological indices are widely used in Quantitative Structure Property Relationship (QSPR) studies. For a molecular graph $G(V, E)$ let $d(u)$ and $d(v)$ denote the degree of vertices $u, v \in V(G)$ respectively and $uv \in E(G)$. The Geometric Arithmetic index is a degree based topological index defined as, $GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{\frac{d(u)+d(v)}{2}}$. Its multiplicative version, called the Multiplicative Geometric Arithmetic index was introduced recently which is defined as, $GAII(G) = \prod_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{\frac{d(u)+d(v)}{2}}$. In this paper, we determine the exact value of $GAII$ for some common polycyclic organic structures, namely graphene, triangular benzenoids, benzenoid series, benzenoid systems and phenylenes. Further we obtain a comparison between GA_1 and $GAII$ indices.

MSC: 05C07, 05C90, 92E10.

Keywords: Molecular graphs, Topological index, Geometric Arithmetic index, Multiplicative Geometric Arithmetic index.

 Accepted on: 13th April 2018

1. Introduction

Graph theoretical concepts are used extensively in chemistry as graphs can be used as effective models to represent chemical molecules. The structure of a molecule can be understood in terms of graphs called molecular graphs. A molecular graph G is a structural representation of the chemical compound in such a way that the atoms form vertices of G, denoted as $V(G)$ and the chemical bonds form the edges of G, denoted as $E(G)$. The characterization of chemical compounds is often not a cost effective process but rather an expensive and time consuming exercise. It has been observed that the molecular structure of compounds is closely related to their physical and chemical properties [2]. Therefore, graph theory provides a convenient way to study and understand properties such as the boiling point, melting point, entropy, heat of formation etc. In particular, graph-theoretical approach has been widely used now in Quantitative Structure Property Relationship (QSPR), a technique that requires only the knowledge of chemical structure. One of the methods to study graphs associated with chemical compounds is to study certain numerical quantities known as *topological indices* that are associated with them. As per the International Union of Pure and Applied Chemistry (IUPAC), topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological

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activity. Mathematically, a topological index can be interpreted as a function that maps a molecular structure of a graph to a positive real number. Over the years several topological indices such as Randić index, Zagreb index, Hosaya index, Atom bond connectivity index, Weiner index and PI index have been introduced in the literature [3–8]. For any graph G let $V(G)$ and $E(G)$ denote the vertex set and edge set of G respectively. The degree of a vertex $u \in V(G)$ is the number of vertices adjacent to u and is denoted as $d(u)$. In this paper we see a variation of the Geometric Arithmetic index that has been introduced by Vukičević and Furtala in [9]. For a graph G, the Geometric Arithmetic index, denoted as $GA_1(G)$ is defined as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{\frac{d(u)+d(v)}{2}}$$

Its multiplicative version was introduced recently in [10] called the Multiplicative Geometric Arithmetic index, denoted as $GAII(G)$ is given by the formula

$$GAII(G) = \prod_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{\frac{d(u)+d(v)}{2}}$$

Though the GA_1 index has been widely studied, the studies related to its multiplicative version is limited. Kulli in [10] calculated the $GAII$ index for some nanotubes. In this paper we determine the $GAII$ index of some organic structures. This is followed by a comparison between GA_1 and $GAII$ indices.

2. Exact Values of $GAII$ Index for Some Polycyclic Organic Structures

In this section we determine the value of $GAII$ index for some polycyclic organic structures, namely graphene, triangular benzenoids, benzenoid series, benzenoid systems and phenylenes. Graphene is a thin layer of carbon that is made up of hexagonal lattice that are stacked one on top of the other. All the chemical compounds that contain a benzene ring are called benzenoid compounds. The circumcoronene is a member of the family of benzenoid compounds, with several benzene rings on its circumference(H_k).

The Capra map operation was first introduced in [15, 16]. When the Capra operation is performed on a benzene (hexagon or C_6), we obtain the Capra designed series of benzenoid ($Ca_k(C_6)$). In [12], we see that the structural characteristics on the perimeter of benzenoid system plays an important role in its properties. These structural characteristics on the perimeter of benzenoid system are, fissures (f), bays(b), coves(C) and fjords(F). Moving along the perimeter of a benzenoid system, the fissure is formed by a vertex of degree 2, followed by vertices of degree 3 and 2 respectively. The bays are formed by vertex of degree 2 followed by two consecutive vertices of degree 3,which is followed by a vertex of degree 2.

The coves and fjords are formed by vertices with degree sequence 2,3,3,3,2 and 2,3,3,3,3,2 respectively. The fissures, bays, coves and fjords are together called inlets, denoted by r. Then the total number of inlets in a benzenoid system is $r = f + b + C + F$. Phenylenes are conjugated, polycyclic benzene rings that are joined together by cyclobutadiene rings [13]. It was observed that the a benzenoid system called hexagonal squeeze had similar properties as that of phenylenes [18–20]. But unlike the benzenoid systems, certain species hexagonal squeeze are helicenic species (geometrically nonplanar). The helicenic species has an another type of structural characteristic on its perimeter called lagoons (L) in addition to fissures, bays, coves and fjords. The lagoon are formed by a sequence of vertices of degrees 2,3,3,3,3,3,2 respectively. Thus the total number of inlets of a helicenic system is $r = f + b + C + F + L$.

Given below are the molecular graphs of these chemical structures. We partition the edge set of G based on the degree of end vertices of edges in order to calculate $GAII$ index. For any $e = uv \in E(G)$, we consider, $E_{a,b} = \{e = uv | d(u) = a \text{ and } d(v) = b\}$.

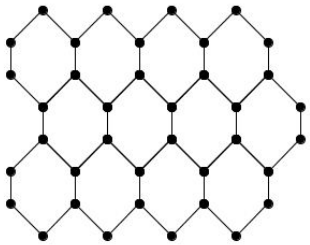

Figure 1. **Molecular graph of 2D lattice structure of graphene with 3 rows and 4 columns**

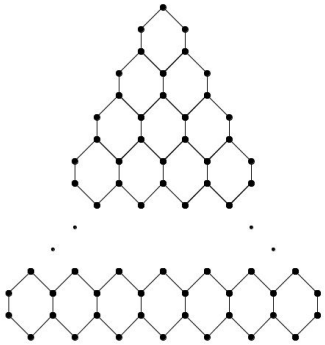

Figure 2. **Molecular graph of Triangular benzenoid.**

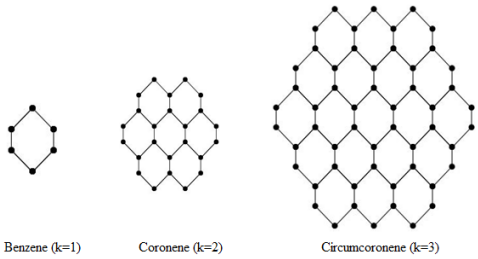

Figure 3. **Molecular graphs, G_{H_1}, G_{H_2}, G_{H_3} from the circumference series of benzenoid.**

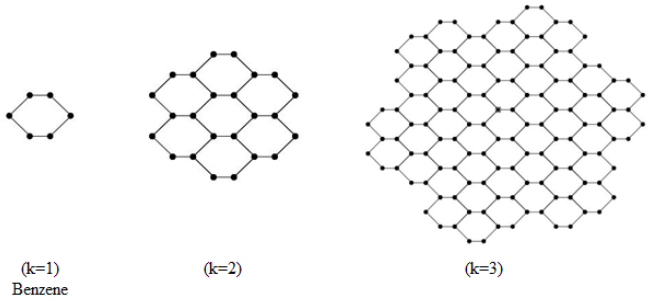

Figure 4. **Molecular graph of $Ca_k(C_6)$, for k= 1, 2 and 3.**

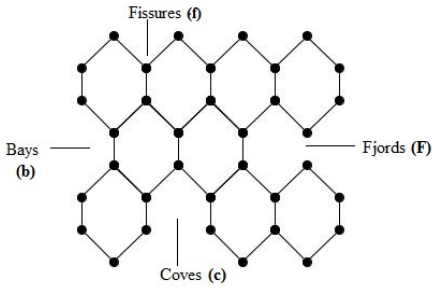

Figure 5. **Molecular graph of a benzenoid system.**

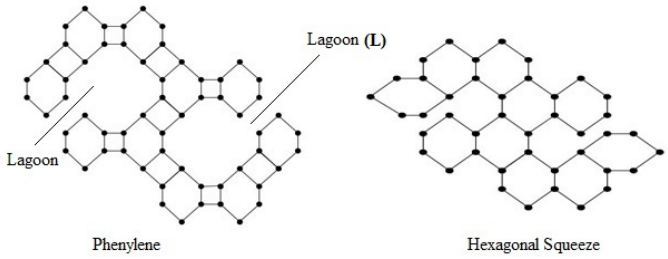

Figure 6. **Molecular graph of a phenylene system and its hexagonal squeeze**

From Figures 1-6, we note that the vertex degrees of the molecular structure under consideration are either 2 or 3. Then the edge set of these structures form a partition into three sets; $E_{2,2}$, consisting of all the edges having end vertices with degree 2; $E_{2,3}$ having the edges with the degrees of its end vertices as 2 and 3 and $E_{3,3}$ consisting of edges with its end vertices of degree 3. Note that $E_{2,3} = E_{3,2}$. Further we note that corresponding to the edges $e = uv$ of $E_{2,2}$ and $E_{3,3}$, value of the expression $\frac{\sqrt{d(u)d(v)}}{\frac{d(u)+d(v)}{2}} = 1$. Hence the value of $GAII$ will be $(\frac{2\sqrt{6}}{5})^{|E_{2,3}|}$. Therefore it is sufficient to determine the $|E_{2,3}|$ for the calculation of $GAII$ index. Table 1 gives the $|E_{2,3}|$ for the chemical structures we have considered.

Molecule	$\lvert E_{2,3}\rvert$
Graphene	$4q + 2p - 4$
Triangular benzenoid	$\frac{3p(p-1)}{2}$
Circumcoronene series	$12(k-1)$
Capra designed series of benzenoid	4.3^k
Benzenoid systems	$2r$
Phenylenes	$2r$

Table 1. **Molecules and cardinality of the corresponding set $E_{2,3}$**

Based on the values we have determined, we compute $GAII$ index of the above mentioned chemical structures, thus leading to the following results.

Result 2.1. *If $G(p,q)$ is a sheet of graphene of p rows and q columns, then $GAII(G(p,q)) = \left(\frac{2\sqrt{6}}{5}\right)^{4q+2p-4}$.*

Result 2.2. *If $G_{t(n)}$ is a triangular benzenoid of p rows, then we have the result $GAII(G_n) = \left(\frac{2\sqrt{6}}{5}\right)^{\frac{3p(p-1)}{2}}$.*

Result 2.3. *For the molecular graph, G_{H_k} of circumcoronene series of benzenoid, $GAII(G_{H_k}) = \left(\frac{2\sqrt{6}}{5}\right)^{12(k-1)}$.*

Result 2.4. *Let $G_{Ca_k(C_6)}$ denote, the capra-designed, planar benzenoid series, then $GAII(G_{Ca_k(C_6)}) = \left(\frac{2\sqrt{6}}{5}\right)^{4.3^k}$.*

Result 2.5. *If G_S denote the benzenoid system, with r inlets, then $GAII(G_S) = \left(\frac{2\sqrt{6}}{5}\right)^{2r}$.*

Result 2.6. *If G_P denote the molecular graph of phenylene with r inlets, we have $GAII(G_P) = \left(\frac{2\sqrt{6}}{5}\right)^{2r}$.*

Remark 2.7. *The graphical structure of Polycyclic Aromatic Hydrocarbons (PAH_n), [14] have degree of its vertices 1 or 3. Using the same approach of partitioning edge set, we find that the $GAII$ index of molecular structure of PAH_n is $(\frac{\sqrt{3}}{2})^{6n}$.*

3. Comparison Between GA_1 and $GAII$ Indices

Knowledge of topological indices become more relevant when a topological index is able to predict the physico-chemical property (properties) of the target molecule. In order to determine if a newly defined topological index is useful in predicting the properties, a comparative study is carried out to determine whether the new index can predict a property of a molecule better than the already existing ones. Here we obtain a comparison between the GA_1 and $GAII$ indices. To avoid the anomalies that occur related to size-dependency, we consider a class of isomers of a chemical compound. Also, to avoid the effects of steric hindrance, polar groups and hydrogen bonding, we consider a class of alkanes, namely octanes. Octanes are the most suitable choice as they have 18 isomers with well defined physico-chemical properties. The benchmark data is collected from [21]. The data contains 16 physico-chemical properties of octanes, such as the Boiling point(BP), Entropy (S), Density ($DENS$), Enthalpy of vaporization ($HVAP$), Standard enthalpy of vaporization ($DHVAP$), Enthalpy of formation ($HFORM$), Acentric factor ($AcenFac$), Molar refraction (MR), etc. For the comparison between GA_1 and $GAII$ indices we find correlation coefficients of GA_1 and $GAII$ indices for the 18 octane isomers with its physico-chemical property. Table 2 presents the GA_1 and $GAII$ indices for the octane isomers whereas Table 3 gives the correlation values of the physico-chemcial properties and GA_1 index and $GAII$ indices.

Molecule	GA_1	$GAII$
n-octane	6.8856	0.8888
2-methyl-heptane	6.6546	0.6928
3-methyl-heptane	6.7112	0.739
4-methyl-heptane	6.7112	0.739
3-ethyl-hexane	6.7678	0.7882
2,2-dimethyl-hexane	6.2856	0.4551
2,3-dimethyl-hexane	6.5206	0.6
2,4-dimethyl-hexane	6.4802	0.576
2,5-dimethyl-hexane	6.4236	0.54
3,3-dimethyl-hexane	6.3712	0.5056
3,4-dimethyl-hexane	6.5772	0.64
2-methyl-3-ethyl-pentane	6.5772	0.64
3-methyl-3-ethyl-pentane	6.4568	0.5618
2,2,3-trimethyl-pentane	6.1783	0.4053
2,2,4-trimethyl-pentane	6.0546	0.3547
2,3,3-trimethyl-pentane	6.2074	0.4222
2,3,4-trimethyl-pentane	6.3301	0.4871
2,2,3,3-tetramethylbutane	5.8	0.2621

Table 2. GA_1 **and** $GAII$ **indices for octane isomers**

Physico-chemical Property	Correlation Coefficients	
	GA_1	$GAII$
BP	**0.8231**	**0.841**
MP	-0.331	-0.3
CV	0.4927	0.4417

Physico-chemical Property	Correlation Coefficients	
CV	-0.153	-0.294
S	**0.9115**	**0.8897**
DENS	-0.553	-0.458
HVAP	**0.9415**	**0.9598**
DHVAP	**0.9655**	**0.9719**
HFORM	**0.8585**	**0.8697**
DHFORM	-0.075	-0.032
MON	0.0974	-0.047
MR	0.5889	0.477
AcenFac	**0.912**	**0.9026**
TSA	0.2445	0.304
Log P	0.1169	0.1823
MV	0.538	0.447

Table 3. **Correlation values of the GA_1 and $GAII$ indices for the physico-chemical properties**

To study the correlation coefficients between GA_1 and $GAII$ indices respectively for the physico-chemical properties, we consider only those properties that give a significantly good correlation respectively for GA_1 and $GAII$ indices. Boiling Point (BP), Entropy (S), Enthalpy of vaporization ($HVAP$), Standard enthalpy of vaporization ($DHVAP$), Enthalpy of formation ($HFORM$) and Acentric Factor ($AcenFac$) are chosen, because GA_1 and $GAII$ indices give correlation coefficients greater than 0.8. Table 4 gives the correlation coefficient between GA_1 and $GAII$ indices with the chosen physico-chemical properties:

Physico-chemical Property	Correlation Coefficient	
	GA_1	$GAII$
BP	0.8231	0.841
S	0.9115	0.8897
HVAP	0.9415	0.9598
DHVAP	0.9655	0.9719
HFORM	0.8585	0.8697
$AcenFac$	0.912	0.9026

Table 4. Correlation coefficients between GA_1 and $GAII$ indices respectively with BP, S, $HVAP$, $DHVAP$, $HFORM$ and $AcenFac$

The graphs showing correlation between the chosen physico-chemical properties and GA_1 and $GAII$ indices respectively are given in Figures 7-12.

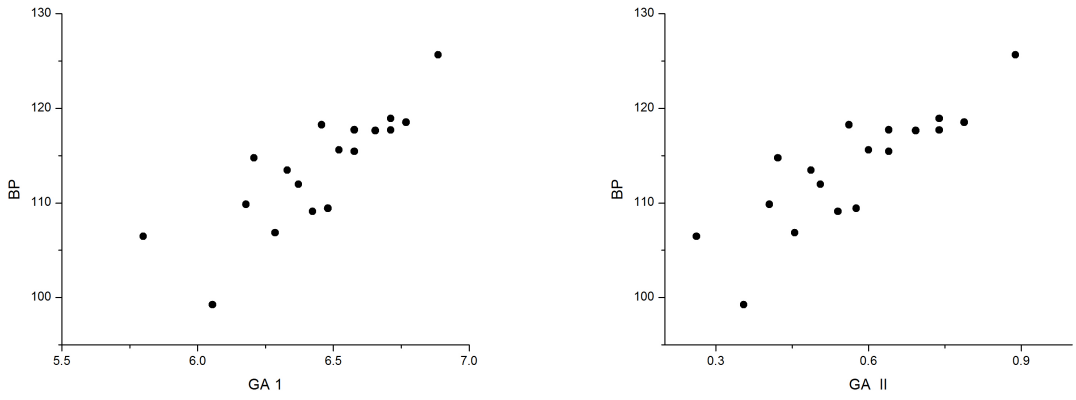

Figure 7. **Graphs of correlation between BP and GA_1, BP and $GAII$ index.**

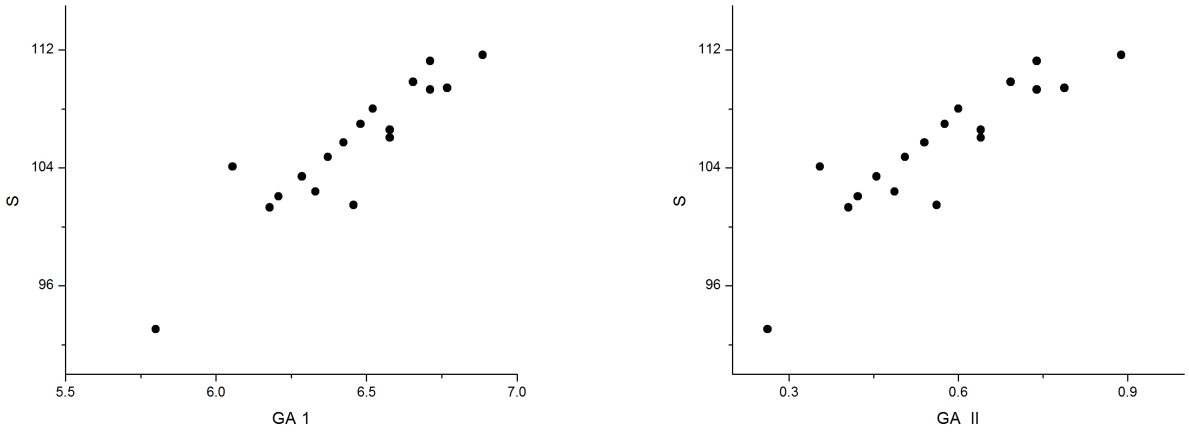

Figure 8. **Graphs of correlation between S and GA_1, S and $GAII$ index.**

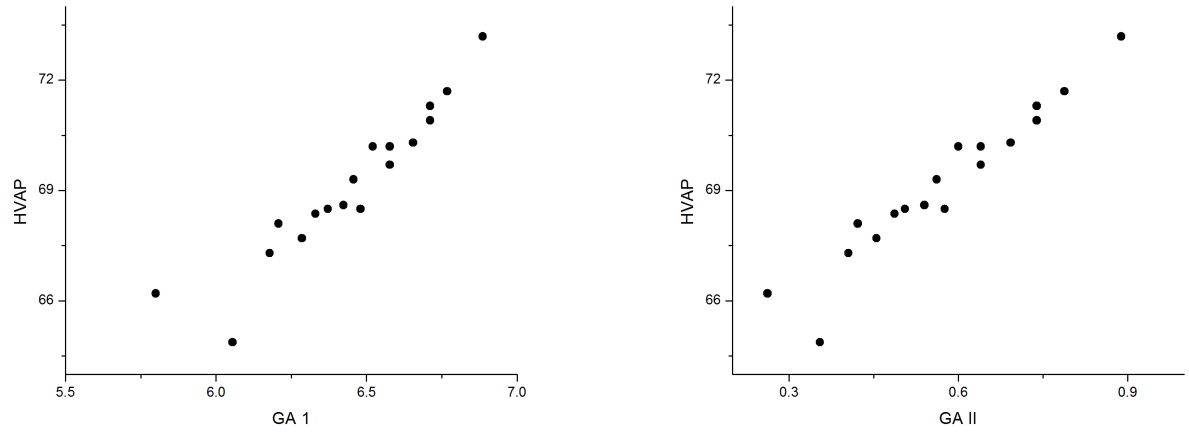

Figure 9. **Graphs of correlation between $HVAP$ and GA_1, $HVAP$ and $GAII$ index.**

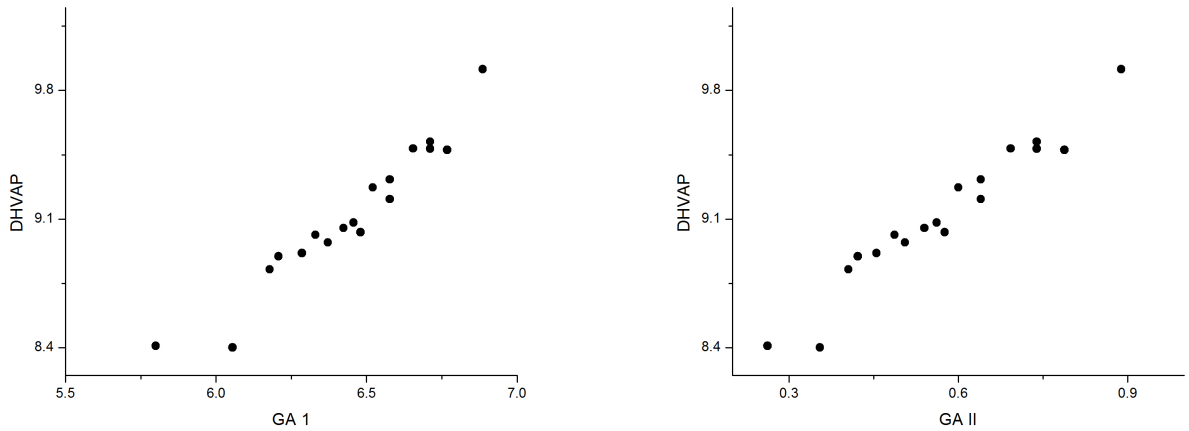

Figure 10. **Graphs of correlation between $DHVAP$ and GA_1, $DHVAP$ and $GAII$ index.**

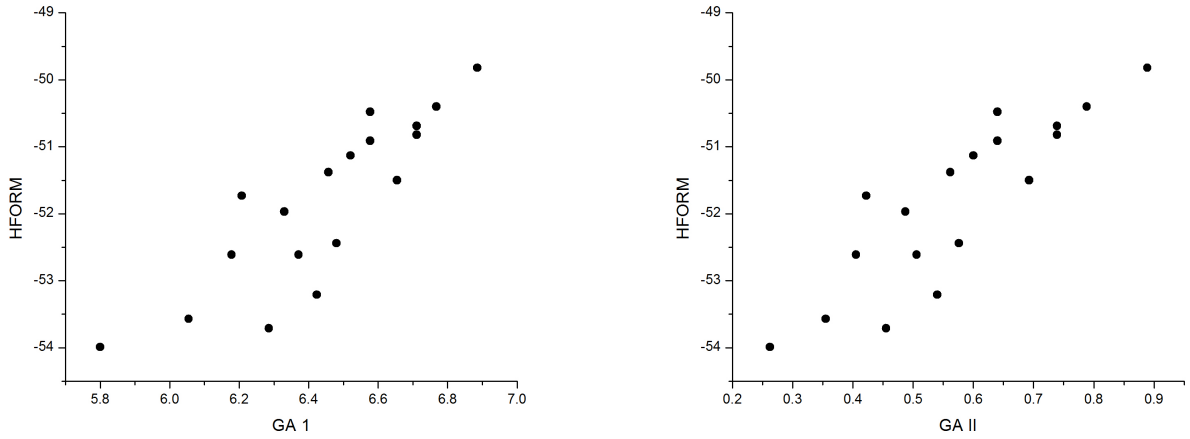

Figure 11. **Graphs of correlation between $HFORM$ and GA_1, $HFORM$ and $GAII$ index.**

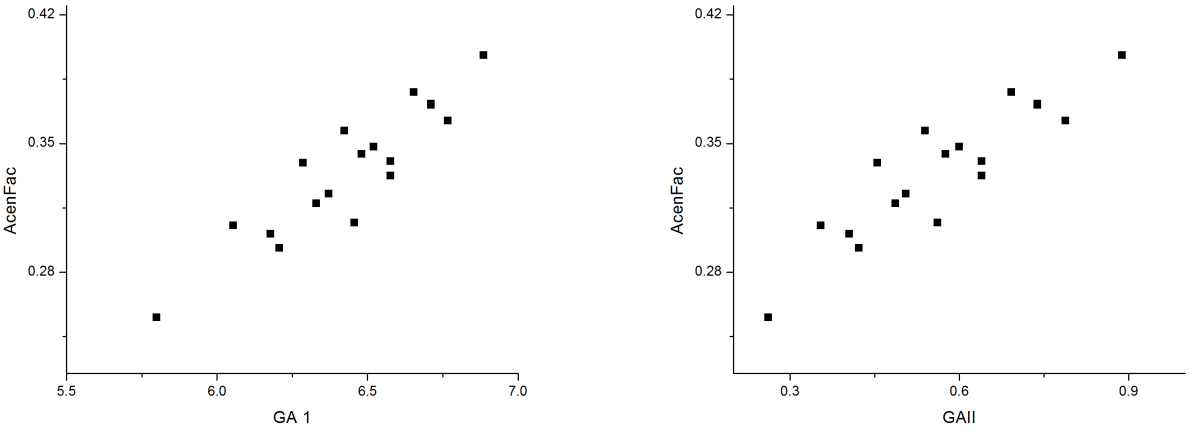

Figure 12. **Graphs of correlation between $AcenFac$ and GA_1, $AcenFac$ and $GAII$ index.**

From the graphical and statistical analysis, we observe that correlation coefficient of $GAII$ index for S and $AcenFac$ is slightly lower than GA_1 index, however we note the correlation coefficient of $GAII$ index is greater than 0.85. In case of BP, $HVAP$, $DHVAP$ and $HFORM$ the corresponding correlation coefficient of $GAII$ index is better than that of GA_1 index and is greater than 0.8. Among correlation coefficients between the $GAII$ index and the chosen physico-chemical properties, it is noted that the correlation coefficient between $GAII$ index and BP has the lowest value of 0.8 and the correlation coefficient between $GAII$ index and $DHVAP$ has the highest value of 0.97. Thus we infer that the predictive ability of $GAII$ index is better than that of GA_1 and is a possible tool for QSPR studies for the physico-chemical properties; boiling point (BP), enthalpy of vaporization ($HVAP$), standard enthalpy of vaporization ($DHVAP$) and enthalpy of formation ($HFORM$).

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