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General Atom-Bond Sum-Connectivity Index of Graphs

Abeer M. Albalahi [1], Emina Milovanović [2] and Akbar Ali [1,*]

[1] Department of Mathematics, College of Science, University of Ha'il, Ha'il P.O. Box 2240, Saudi Arabia
[2] Faculty of Electronic Engineering, University of Niš, 18000 Niš, Serbia
* Correspondence: akbarali.maths@gmail.com

Abstract: This paper is concerned with the general atom-bond sum-connectivity index ABS_γ, which is a generalization of the recently proposed atom-bond sum-connectivity index, where γ is any real number. For a connected graph G with more than two vertices, the number $ABS_\gamma(G)$ is defined as the sum of $(1 - 2(d_x + d_y)^{-1})^\gamma$ over all edges xy of the graph G, where d_x and d_y represent the degrees of the vertices x and y of G, respectively. For $-10 \le \gamma \le 10$, the significance of ABS_γ is examined on the data set of twenty-five benzenoid hydrocarbons for predicting their enthalpy of formation. It is found that the predictive ability of the index ABS_γ for the selected property of the considered hydrocarbons is comparable to other existing general indices of this type. The effect of the addition of an edge between two non-adjacent vertices of a graph under ABS_γ is also investigated. Furthermore, several extremal results regarding trees, general graphs, and triangle-free graphs of a given number of vertices are proved.

Keywords: general atom-bond sum-connectivity; topological index; tree graph; chemical graph theory; triangle-free graph

MSC: 05C07; 05C90

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1. Introduction

A property of a graph that is preserved by the graph isomorphism is known as a graph invariant (see [1]). The real-valued graph invariants are frequently referred to as topological indices. The readers are referred to [1–3] for (chemical) graph theory terminology and notations.

The connectivity index (often referred to as the Randić index, which was initially developed in [4] with name "branching index") has taken a significant position among the most studied and implemented topological indices. The connectivity index is thought to be the topological index that has been studied the most, in terms of theory as well as implementation, according to [5]. This index for a graph G is represented by the following number:

$$R(G) = \sum_{st \in E(G)} \frac{1}{\sqrt{d_s d_t}},$$

where d_v stands for the degree of a vertex v in G, and $E(G)$ stands for the edge set of G. (If more than one graph is being considered, we express the degree of v in G using the notion $d_v(G)$ to prevent confusion). More details on the research of the connectivity index may be found in the survey papers [6,7], books [8,9], and related works cited therein.

The scientific literature now contains a number of variants of the connectivity index due to its growing popularity. The sum-connectivity (SC) index [10] and the atom-bond connectivity (ABC) index [11,12] are two of the variants of the connectivity index that have been the subject of substantial investigation; these indices have the following definitions

$$SC(G) = \sum_{st \in E(G)} \frac{1}{\sqrt{d_s + d_t}}$$

and

$$ABC(G) = \sum_{st \in E(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}}.$$

The SC index's fundamental idea was used in [13] to produce the atom-bond sum-connectivity (ABS) index, a new variation of the ABC index. The ABS index of a graph G is defined as

$$ABS(G) = \sum_{st \in E(G)} \sqrt{1 - \frac{2}{d_s + d_t}}.$$

In [13], certain extremal results about the ABS index of (chemical) trees and general graphs were reported. Article [14] not only gives a solution to an extremal problem involving the ABS index for unicyclic graphs, but it also reports chemical uses of the ABS index. The trees with the lowest ABS index were examined in [15,16] independently, with a specified number of vertices of degree 1 and a fixed order. Further existing results on the ABS index can be found in [17–19].

The general ABS index [14] for a graph G is defined as

$$ABS_\gamma(G) = \sum_{st \in E(G)} \left(1 - \frac{2}{d_s + d_t}\right)^\gamma,$$

where γ can assume any real number with the constraint that the graph G must satisfy the following property when $\gamma < 0$: $d_s + d_t > 2$ for every edge $st \in E(G)$. Note that if the inequality $d_s + d_t > 2$ holds for every $st \in E(G)$, then $ABS_\gamma(G)$ can also be defined as

$$ABS_\gamma(G) = \sum_{st \in E(G)} \left(1 + \frac{2}{d_{st}}\right)^{-\gamma},$$

where $d_{st} = d_s + d_t - 2$, which is the degree of the edge st. Here, we highlight that the general ABS index (and subsequently the ABS index) is a special case of a more general topological index that was first investigated in [20].

In the upcoming section, the chemical usefulness of ABS_γ is examined on the data set of twenty-five benzenoid hydrocarbons for predicting their enthalpy of formation for $-10 \le \gamma \le 10$; it was found that the predictive ability of the index ABS_γ for the selected property of the considered hydrocarbons is comparable to other existing general indices of this type. Investigating the impact of the addition of an edge in a non-complete graph under ABS_γ is the focus of Section 3, where a non-complete graph is one that differs from the complete graph. In Section 4, a number of extremal problems about trees, general graphs, and triangle-free graphs of a given number of vertices are addressed.

2. Chemical Applicability of ABS_γ

In the current section, the significance of ABS_γ is examined on the data set of twenty-five benzenoid hydrocarbons (having names given in Table 1) for predicting the enthalpy of formation ΔH_f of the mentioned hydrocarbons for $-10 \le \gamma \le 10$. The experimental data (given in Table 1) for the selected property of these hydrocarbons is taken from [21,22].

First, we calculate the ABS, ABC, SC and R indices of molecular graphs of the twenty-five benzenoid hydrocarbons under consideration. For doing this, we establish a general expression for evaluating the aforementioned indices. By a hexagonal system, we mean a molecular graph of a benzenoid hydrocarbon. In a hexagonal system, a vertex of degree 3 lying on three hexagons is known as an internal vertex; a vertex that is not an internal vertex is referred to as an external vertex. In addition, in a hexagonal system, an edge whose both end vertices are incident to external vertices is called an external edge; an edge that is not an external edge is known as an internal edge. For example, see Figure 1 where internal/external vertices are indicated by black/white vertices, respectively, while internal/external edges are indicated by thin/bold edges, respectively. A hexagonal system possessing no internal vertex is commonly referred to as a catacondensed hexagonal system. In a catacondensed hexagonal system, an edge whose every vertex has degree 3 is referred to as a branched hexagon. By a kink in a catacondensed hexagonal system, we mean a hexagon possessing exactly one pair of adjacent vertices of degree 2. For further information regarding hexagonal systems, the readers are referred to [23].

Table 1. The values of the enthalpy of formation ΔH_f and the indices ABS, ABC, SC, R, for the considered 25 hydrocarbons.

Compound Name	ABS	ABC	R	SC	ΔH_f
benzene	4.2426	4.2426	3.0000	3.0000	82.9
naphthalene	8.1575	7.7377	4.9663	5.1971	150.6
anthracene	12.0724	11.2328	6.9327	7.3942	227.7
phenanthrene	12.0468	11.1924	6.9495	7.4080	207.1
pyrene	14.5219	13.2328	7.9327	8.6190	225.7
benzo[a]anthracene	15.9617	14.6875	8.9158	9.6051	291.0
benzo[c]phenanthrene	15.9361	14.6470	8.9327	9.6190	302.4
chrysene	15.9361	14.6470	8.9327	9.6190	262.8
naphthacene	15.9873	14.7279	8.8990	9.5913	291.4
triphenylene	15.9105	14.6066	8.9495	9.6328	269.8
benzo[a]pyrene	18.4112	16.6875	9.9158	10.8299	301.0
benzo[e]pyrene	18.3856	16.6470	9.9327	10.8437	304.0
perylene	18.3856	16.6470	9.9327	10.8437	324.0
benzo[b]chrysene	19.8510	18.1421	10.8990	11.8161	346.0
benzo[c]chrysene	19.8254	18.1017	10.9158	11.8299	334.0
benzo[g]chrysene	19.7998	18.0613	10.9327	11.8437	333.0
benzo[a]tetracene	19.8766	18.1826	10.8821	11.8022	359.0
dibenzo[a,c]anthracene	19.8254	18.1017	10.9158	11.8299	345.0
dibenzo[a,h]anthracene	19.8510	18.1421	10.8990	11.8161	343.0
dibenzo[a,j]anthracene	19.8510	18.1421	10.8990	11.8161	343.0
dibenzo[b,g]phenanthrene	19.8510	18.1421	10.8990	11.8161	347.0
dibenzo[c,g]phenanthrene	19.8254	18.1017	10.9158	11.8299	335.0
pentacene	19.9022	18.2230	10.8653	11.7884	374.5
pentaphene	19.8766	18.1826	10.8821	11.8022	359.0
picene	19.8254	18.1017	10.9158	11.8299	334.0

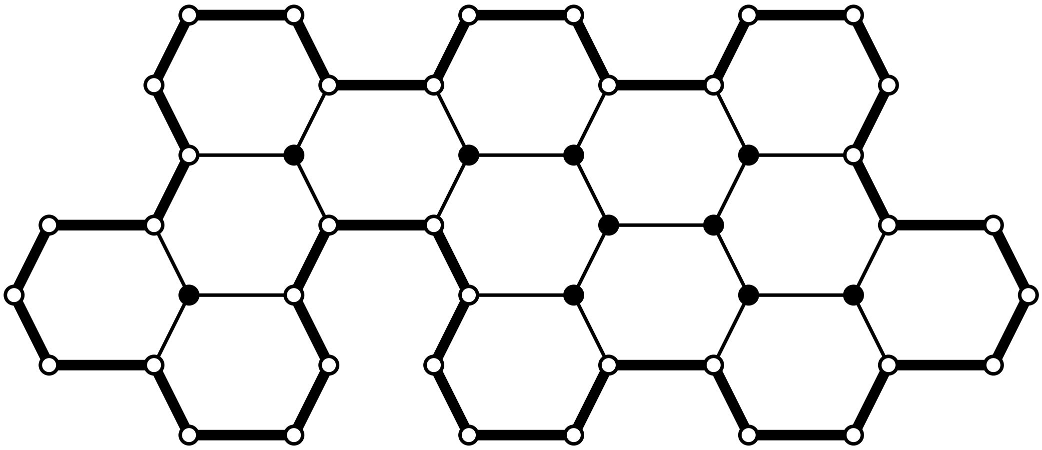

Figure 1. A hexagonal system differentiating internal and external vertices/edges.

Let H_h be any catacondensed hexagonal system possessing h hexagons, from which h_k are kinks and h_b are branched hexagons. Then, one has

$$m_{2,2}(H_h) = 3h_b + h_k + 6, \;\; m_{2,3}(H_h) = 2(2h - 3h_b - h_k - 2), \;\text{ and}$$

$$m_{3,3}(H_h) = 3h_b + h_k + h - 1,$$

where $m_{i,j}(H_h)$ is the cardinality of the set

$$\{st \in E(H_h) : d_t = j, \; d_s = i\}.$$

Thus, by making use of the formula of ABS_γ, we have

$$\begin{aligned} ABS_\gamma(H_h) = {} & (3h_b + h_k + 6)\left(\frac{1}{2}\right)^\gamma + 2(2h - 3h_b - h_k - 2)\left(\frac{3}{5}\right)^\gamma \\ & + (3h_b + h_k + h - 1)\left(\frac{2}{3}\right)^\gamma, \end{aligned}$$

which is equivalent to

$$\begin{aligned} ABS_\gamma(H_h) = {} & \left(4\left(\frac{3}{5}\right)^\gamma + \left(\frac{2}{3}\right)^\gamma\right)h + \left(\left(\frac{1}{2}\right)^\gamma - 2\left(\frac{3}{5}\right)^\gamma + \left(\frac{2}{3}\right)^\gamma\right)h_k \\ & + 3\left(\left(\frac{1}{2}\right)^\gamma - 2\left(\frac{3}{5}\right)^\gamma + \left(\frac{2}{3}\right)^\gamma\right)h_b \\ & + 6\left(\frac{1}{2}\right)^\gamma - 4\left(\frac{3}{5}\right)^\gamma - \left(\frac{2}{3}\right)^\gamma. \end{aligned} \tag{1}$$

The value of $ABS_\gamma(H_h)$ can be calculated by utilizing Formula (1). By utilizing the obtained information about the number of edges of different types in any catacondensed hexagonal system, we now derive a general version of (1). A bond incident degree (BID) index of H_h is defined as

$$BID(H_h) = \sum_{2 \le i \le j \le 3} m_{i,j}(H_h) \cdot \beta_{i,j}\,, \tag{2}$$

which implies that

$$\begin{aligned} BID(H_h) = {} & (3h_b + h_k + 6)\beta_{2,2} + 2(2h - 3h_b - h_k - 2)\beta_{2,3} \\ & + (3h_b + h_k + h - 1)\beta_{3,3}, \end{aligned}$$

which is equivalent to

$$BID(H_h) = (4\beta_{2,3} + \beta_{3,3})h + (\beta_{2,2} - 2\beta_{2,3} + \beta_{3,3})h_k + 3(\beta_{2,2} - 2\beta_{2,3} + \beta_{3,3})h_b + 6\beta_{2,2} - 4\beta_{2,3} - \beta_{3,3}. \quad (3)$$

Now, we calculate the ABS, ABC, SC and R indices of molecular graphs of the benzenoid hydrocarbons having names given in Table 1 (the calculated values of the mentioned indices are also given in the same table); we remark here that most of these molecular graphs are catacondensed hexagonal systems, and hence, the mentioned indices are calculated by utilizing (3).

Now, we calculate the correlation coefficient between ΔH_f and the ABS, ABC, SC and R indices for the hydrocarbons mentioned in Table 1. From Table 2, it follows that all the four examined indices perform almost the same in predicting the enthalpy of formation of the hydrocarbons mentioned in Table 1.

Table 2. The positive value of the correlation coefficient between the enthalpy of formation and the ABS, ABC, SC and R indices for the hydrocarbons mentioned in Table 1.

	ABS	***ABC***	***R***	***SC***
Enthalpy of formation	0.9806	0.9826	0.9823	0.9815

If $\beta_{i,j} = ((i+j-2)/ij)^\gamma$ or $\beta_{i,j} = (i+j))^\gamma$ or $\beta_{i,j} = (ij))^\gamma$, then Equation (2) yields ABC_γ or the sum-connectivity index SC_γ or the general Randić index R_γ, respectively. Next, we calculate the correlation coefficient between ΔH_f and ABS_γ, ABC_γ, SC_γ, R_γ for the hydrocarbons mentioned in Table 1. The positive values for the correlation r (between the selected property of the considered hydrocarbons and ABS_γ, ABC_γ, SC_γ, R_γ), with $\gamma \in [-10, 10]$, are depicted in Figures 2–5. The maximum positive values for the correlation r (between the selected property of the considered hydrocarbons and ABS_γ, ABC_γ, SC_γ, R_γ), with $\gamma \in [-10, 10]$, are given in Table 3. Table 3 indicates that the maximum positive values for the correlation r of the examined four indices are neither considerably different from one another nor significantly better than the ones given in Table 2.

Table 3. The maximum positive value for the correlation r, between ΔH_f of the considered hydrocarbons and the considered topological indices (that are ABS_γ, ABC_γ, SC_γ and R_γ), when $\gamma \in [-10, 10]$.

Index	**Correlation (*r*)**	γ
ABS_γ	0.9869	-0.1626
ABC_γ	0.9903	6.07095
SC_γ	0.9815	-0.6431
R_γ	0.9823	-0.4818

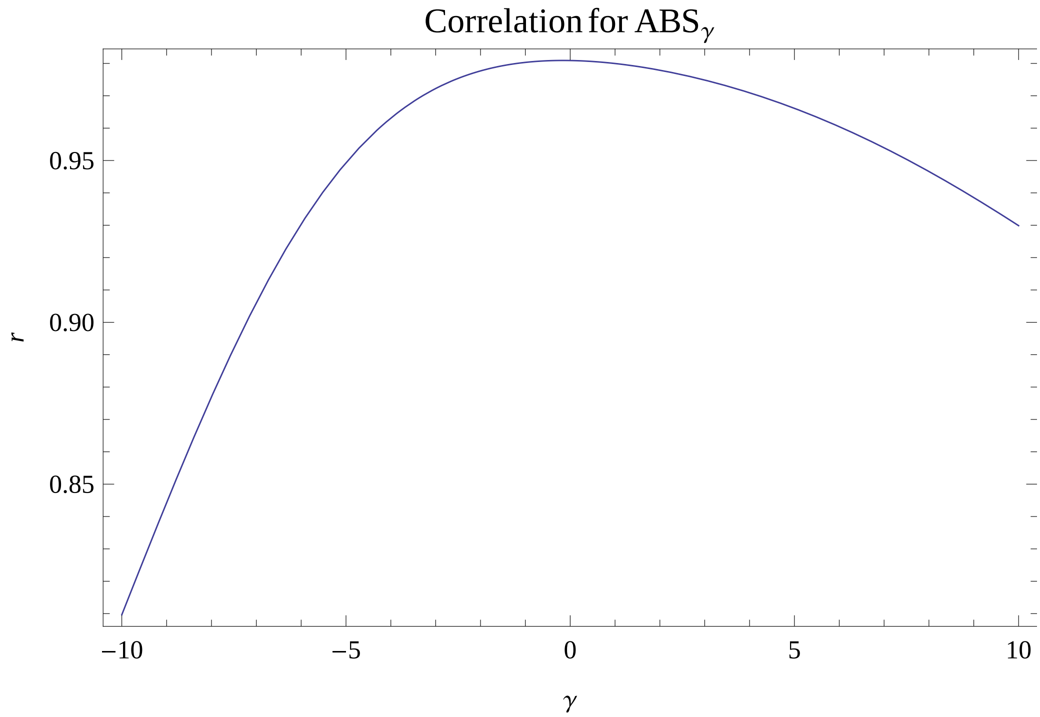

Figure 2. The positive value for the correlation R (between ΔH_f of the considered hydrocarbons and ABS_γ) for $\gamma \in [-10, 10]$.

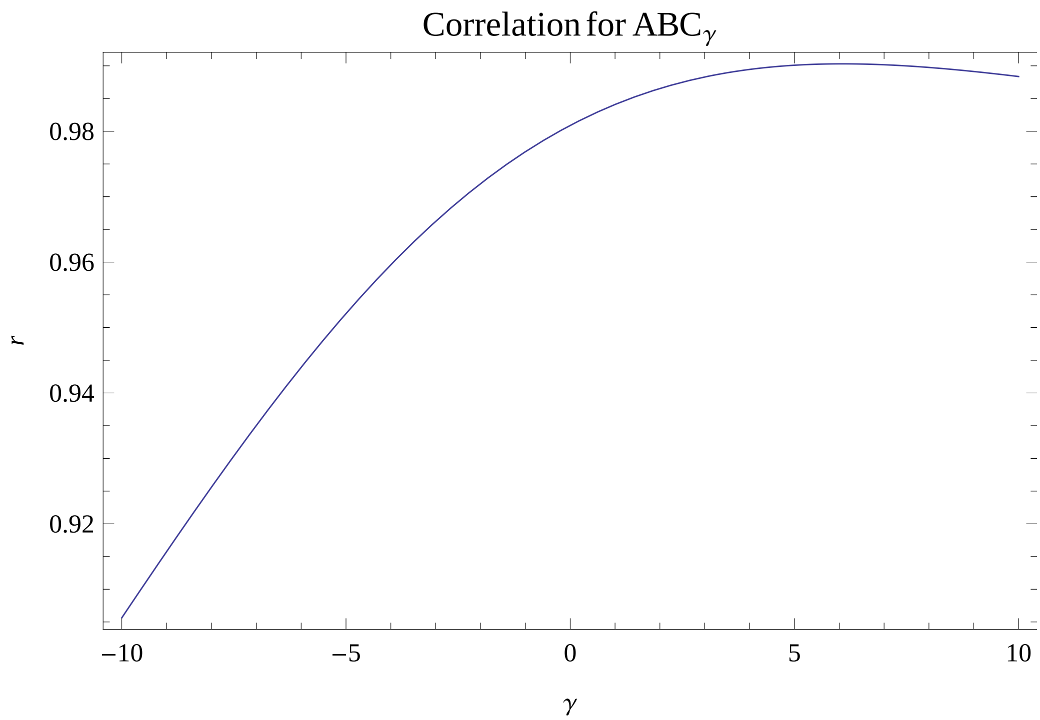

Figure 3. The positive value for the correlation R (between ΔH_f of the considered hydrocarbons and ABC_γ) for $\gamma \in [-10, 10]$.

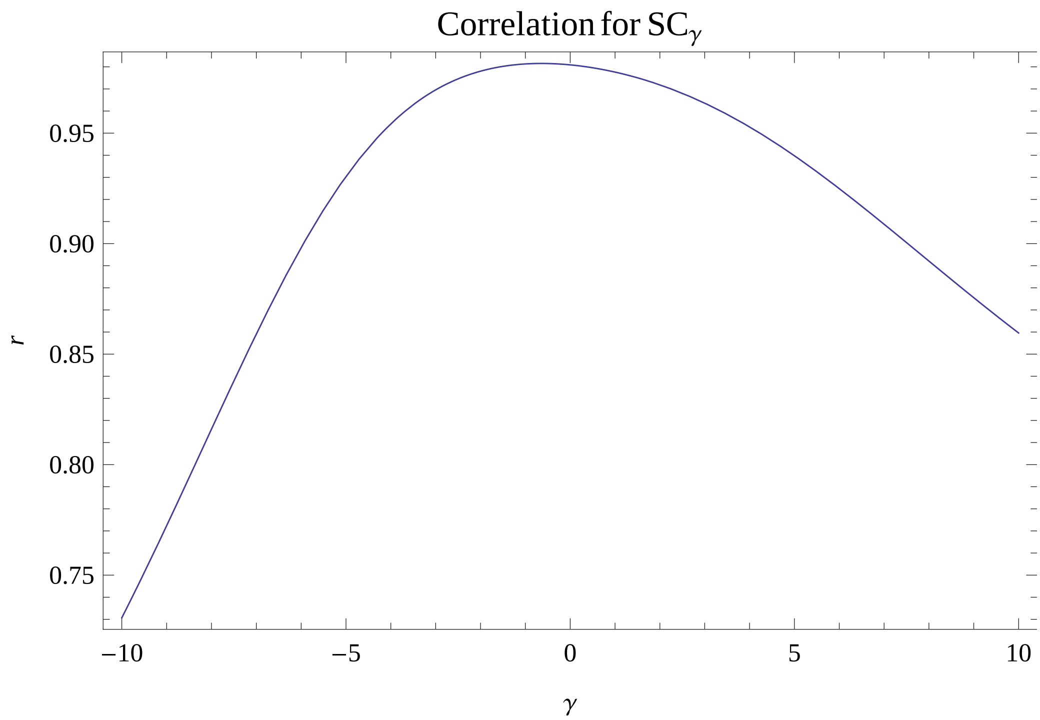

Figure 4. The positive value for the correlation R (between ΔH_f of the considered hydrocarbons and SC_γ) for $\gamma \in [-10, 10]$.

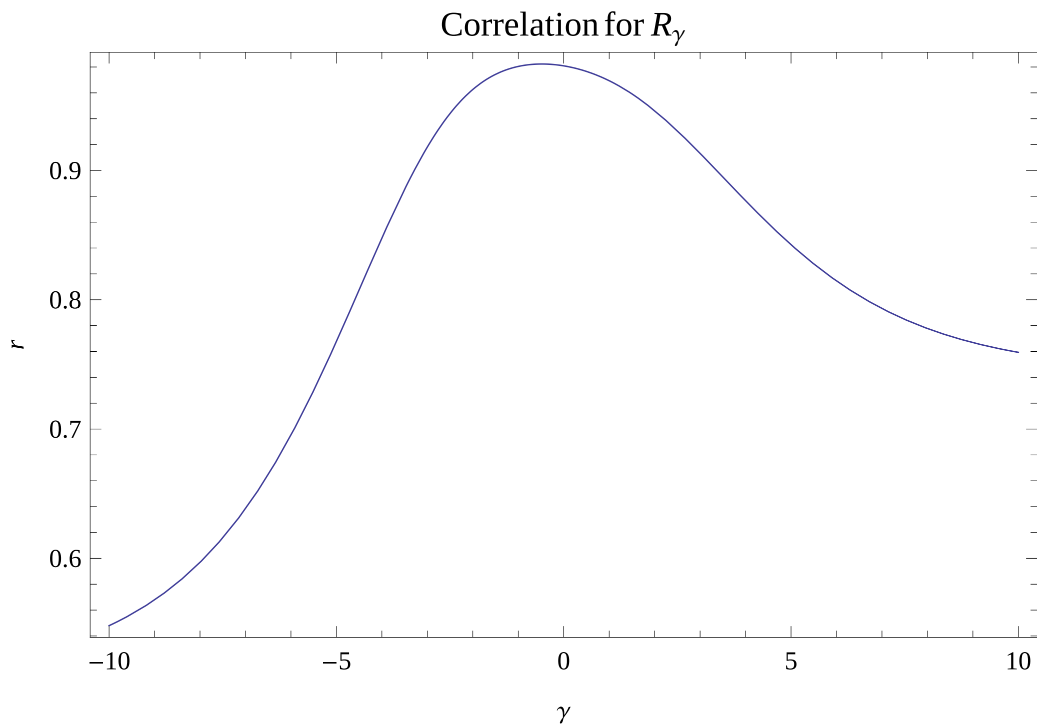

Figure 5. The positive value for the correlation R (between ΔH_f of the considered hydrocarbons and R_γ) for $\gamma \in [-10, 10]$.

3. Behavior of ABS_γ Under the Addition of an Edge

Let G be a graph such that $st \notin E(G)$. By the graph $G + st$, we mean the graph formed by adding the edge st in G. In this section, it is proved that $ABS_\gamma(G + st) > ABS_\gamma(G)$ whenever $\gamma \geq 0$. The following already existing result is required to prove the aforementioned inequality involving ABS_γ.

Lemma 1 ([13]). *Let φ be a strictly increasing function of two variables α and β with the constraints $\varphi(\alpha,\beta)=\varphi(\beta,\alpha)\geq 0$, $\alpha\geq 1$ and $\beta\geq 1$. If s and t are non-adjacent vertices in a graph G such that $\max\{d_s,d_t\}\geq 1$, then*

$$\sum_{st\in E(G+st)}\varphi\big(d_s(G+st),d_t(G+st)\big)>\sum_{st\in E(G)}\varphi\big(d_s(G),d_t(G)\big).$$

Proposition 1. *If s and t are non-adjacent vertices in a graph G such that $\max\{d_s,d_t\}\geq 1$, then*

$$ABS_\gamma(G+st)>ABS_\gamma(G)$$

for $\gamma\geq 0$.

Proof. If $\gamma=0$, then we have

$$ABS_\gamma(G+st)=|E(G)|+1>|E(G)|=ABS_\gamma(G).$$

Next, suppose that $\gamma>0$. Certainly, the function ψ with the following definition is strictly increasing for $\gamma>0$:

$$\psi(\alpha,\beta)=\left(1-\frac{2}{\alpha+\beta}\right)^{\gamma}.$$

Thus, Lemma 1 guaranties the desired conclusion. □

4. Extremal Results

This section is devoted to proving several extremal results concerning trees, general graphs, and triangle-free graphs of a given order. The following lemma is very crucial in proving the first main result of this section.

Lemma 2. *For a fixed positive real number γ greater than or equal to $\frac{2}{5}$, define a function ψ_γ as*

$$\psi_\gamma(\alpha)=2\left(\frac{\alpha}{\alpha+2}\right)^{\gamma}-\left(\frac{\alpha-1}{\alpha+1}\right)^{\gamma},$$

where $\alpha\geq 3$. The function ψ_γ is strictly increasing.

Proof. Throughout the proof, it is assumed that $\alpha\geq 3$. The derivative function ψ'_γ of ψ_γ is determined as

$$\psi'_\gamma=2\gamma\left(\frac{2\alpha^{\gamma-1}}{(\alpha+2)^{\gamma+1}}-\frac{(\alpha-1)^{\gamma-1}}{(\alpha+1)^{\gamma+1}}\right).$$

In order to prove the result, it is enough to show that

$$\frac{2\alpha^{\gamma-1}}{(\alpha+2)^{\gamma+1}}>\frac{(\alpha-1)^{\gamma-1}}{(\alpha+1)^{\gamma+1}}\quad\text{for } \gamma\geq\frac{2}{5},$$

or

$$2\left(\frac{\alpha}{\alpha-1}\right)^{\gamma-1}>\left(\frac{\alpha+2}{\alpha+1}\right)^{\gamma+1}\quad\text{for } \gamma\geq\frac{2}{5},$$

which is equivalent to

$$\ln 2>(\gamma+1)\Big(\ln(\alpha+2)-\ln(\alpha+1)\Big)-(\gamma-1)\Big(\ln\alpha-\ln(\alpha-1)\Big),\tag{4}$$

for $\gamma\geq\frac{2}{5}$. In what follows, we prove (4).

The mean value theorem confirms the existence of the numbers a_1 and a_2 with $\alpha - 1 < a_1 < \alpha$ and $\alpha + 1 < a_2 < \alpha + 2$ such that

$$(\gamma+1)\Big(\ln(\alpha+2)-\ln(\alpha+1)\Big)-(\gamma-1)\Big(\ln\alpha-\ln(\alpha-1)\Big)$$
$$=\frac{\gamma+1}{a_2}-\frac{\gamma-1}{a_1} \tag{5}$$

If $\gamma = 1$, then

$$\frac{\gamma+1}{a_2}-\frac{\gamma-1}{a_1}<\frac{2}{\alpha+1}<\ln 2 \tag{6}$$

(because $a_2 > \alpha + 1$) and thence from (5) and (6), the inequality (4) follows.

If $\frac{2}{5} \leq \gamma < 1$, then

$$\begin{aligned}\frac{\gamma+1}{a_2}-\frac{\gamma-1}{a_1}&<\frac{\gamma+1}{\alpha+1}-\frac{\gamma-1}{\alpha-1}\\&=\frac{2(\alpha-\gamma)}{\alpha^2-1}\\&\leq\frac{2(\alpha-\frac{2}{5})}{\alpha^2-1}<\ln 2.\end{aligned} \tag{7}$$

(because $a_2 > \alpha + 1$ and $a_1 > \alpha - 1$) and thence from (5) and (7), the inequality (4) follows.

Finally, if $\gamma > 1$, then

$$\frac{\gamma+1}{a_2}-\frac{\gamma-1}{a_1}<\frac{\gamma+1}{\alpha+1}-\frac{\gamma-1}{\alpha}<\frac{\gamma+1}{\alpha}-\frac{\gamma-1}{\alpha}=\frac{2}{\alpha}<\ln 2 \tag{8}$$

(because $a_2 > \alpha + 1$ and $a_1 < \alpha$) and thence from (5) and (8), the inequality (4) follows. □

The following elementary lemma is also used in the proof of the first main result (that is Theorem 1) of this section.

Lemma 3. *For every positive (negative) real number γ, the function ϕ_γ defined below is strictly increasing (decreasing, respectively) in both α and β*

$$\phi_\gamma(\alpha,\beta)=\left(1-\frac{2}{\alpha+\beta}\right)^\gamma,$$

where $\min\{\alpha,\beta\} \geq 1$.

Let $P : x_1 \cdots x_k$ be a non-trivial path in a graph G. The path P is pendent if and only if $\max\{d_{x_1}, d_{x_k}\} \geq 3$, $\min\{d_{x_1}, d_{x_k}\} = 1$ and $d_{x_i} = 2$ when $2 \leq i \leq k-1$. Two pendent paths of a graph are said to be adjacent if they have a vertex in common.

Theorem 1. *For $\gamma \geq \frac{2}{5}$, if H is a graph with a minimum value of ABS_γ in the family of all connected graphs of size m and order n, then the graph H possess no adjacent pendent paths.*

Proof. We prove the contra-positive statement of the theorem. Assume that $P : ca_1 \cdots a_r$ and $P' : cb_1 \cdots b_s$ are adjacent pendent paths in H, where a_r and b_s are pendent vertices, and $d_c \geq 3$. Denote by H' the graph deduced from H by dropping the edge b_1c and by adding the edge b_1a_r. Obviously, $V(H) = V(H')$ and $|E(H)| = |E(H')|$. In the following, we show that the inequality $ABS_\gamma(H) > ABS_\gamma(H')$ holds, which gives the conclusion of the contra-positive statement of the theorem. Take $X = N_H(a) \setminus \{a_1, b_1\}$ and assume that $\gamma \geq \frac{2}{5}$.

Case 1. $r = s = 1$.
By utilizing the definition of ABS_γ and Lemma 3, one has

$$\begin{aligned} ABS_\gamma(H) - ABS_\gamma(H') = &\sum_{x \in X} \left(\left(1 - \frac{2}{d_c + d_x}\right)^\gamma - \left(1 - \frac{2}{d_c + d_x - 1}\right)^\gamma \right) \\ &+ \left(1 - \frac{2}{d_c + 1}\right)^\gamma - \left(\frac{1}{3}\right)^\gamma > 0. \end{aligned}$$

Case 2. $\max\{r, s\} \geq 2$ and $\min\{r, s\} = 1$.
In this case, again one obtains

$$\begin{aligned} ABS_\gamma(H) - ABS_\gamma(H') = &\sum_{x \in X} \left(\left(1 - \frac{2}{d_c + d_x}\right)^\gamma - \left(1 - \frac{2}{d_c + d_x - 1}\right)^\gamma \right) \\ &+ \left(1 - \frac{2}{d_c + 2}\right)^\gamma - \left(\frac{1}{2}\right)^\gamma > 0. \end{aligned}$$

Case 3. $\min\{r, s\} \geq 2$.
In this case, by using Lemma 3, we have

$$\begin{aligned} ABS_\gamma(H) - ABS_\gamma(H') = &\sum_{x \in X} \left(\left(1 - \frac{2}{d_c + d_x}\right)^\gamma - \left(1 - \frac{2}{d_c + d_x - 1}\right)^\gamma \right) \\ &+ 2\left(1 - \frac{2}{d_c + 2}\right)^\gamma - \left(1 - \frac{2}{d_c + 1}\right)^\gamma \\ &+ \left(\frac{1}{3}\right)^\gamma - 2\left(\frac{1}{2}\right)^\gamma \\ > &\, 2\left(1 - \frac{2}{d_c + 2}\right)^\gamma - \left(1 - \frac{2}{d_c + 1}\right)^\gamma \\ &+ \left(\frac{1}{3}\right)^\gamma - 2\left(\frac{1}{2}\right)^\gamma. \end{aligned} \tag{9}$$

Now, by using Lemma 2 on the right-hand side of Equation (9), we obtain

$$ABS_\gamma(H) - ABS_\gamma(H') > 2\left(\frac{3}{5}\right)^\gamma + \left(\frac{1}{3}\right)^\gamma - 3\left(\frac{1}{2}\right)^\gamma > 0.$$

as needed. □

Theorem 1 directly implies the following result.

Corollary 1. *For $\gamma \geq \frac{2}{5}$ and $n \geq 3$, if G is any n-vertex tree graph different from the path graph P_n, then*

$$ABS_\gamma(G) > (n-3)\left(\frac{1}{2}\right)^\gamma + 2\left(\frac{1}{3}\right)^\gamma = ABS_\gamma(P_n).$$

Proposition 1 and Theorem 1 directly imply the following result.

Corollary 2. *For $\gamma \geq \frac{2}{5}$ and $n \geq 4$, if G is any connected n-vertex graph different from the path and complete graphs P_n, K_n, then*

$$\begin{aligned} ABS_\gamma(P_n) = (n-3)\left(\frac{1}{2}\right)^\gamma + 2\left(\frac{1}{3}\right)^\gamma &< ABS_\gamma(G) \\ &< \binom{n}{2}\left(\frac{n-2}{n-1}\right)^\gamma = ABS_\gamma(K_n). \end{aligned}$$

Theorem 2. *Let G be a graph. Let $xy \in E(G)$ such that xy is not a part of any triangle (if it exists) of G and $d_x \geq d_y \geq 2$. Take $N_G(y) = \{y_1, y_2, \ldots, y_{d_y-1}, x\}$ and $N_G(x) = \{x_1, x_2, \ldots, x_{d_x-1}, y\}$. Generate a graph $G^\star$ from G by dropping out the edges $y_1y, y_2y, \cdots, y_ry$ and by inserting $x_1y, x_2y, \cdots, x_ry$. Then, $ABS_\gamma(G) < ABS_\gamma(G^\star)$ for $\gamma > 0$ and $ABS_\gamma(G) > ABS_\gamma(G^\star)$ for $\gamma < 0$*

Proof. By making use of the definition of ABS_γ, one obtains

$$\begin{aligned}
&ABS_\gamma(G) - ABS_\gamma(G^\star)\\
&= \sum_{i=1}^{d_x(G)-1}\left(\left(1 - \frac{2}{d_x(G) + d_{x_i}(G)}\right)^\gamma - \left(1 - \frac{2}{d_x(G) + d_{x_i}(G) + d_y(G) - 1}\right)^\gamma\right)\\
&+ \sum_{j=1}^{d_y(G)-1}\left(\left(1 - \frac{2}{d_y(G) + d_{y_i}(G)}\right)^\gamma - \left(1 - \frac{2}{d_x(G) + d_{y_i}(G) + d_y(G) - 1}\right)^\gamma\right);
\end{aligned}$$

the right-hand side of this equation is negative for $\gamma > 0$ and positive for $\gamma < 0$, because of Lemma 3. □

Theorem 3. *For $n \geq 4$, if G is any n-vertex tree graph different from the star graph S_n, then*

$$ABS_\gamma(G)\begin{cases} < (n-1)\left(\dfrac{n-2}{n}\right)^\gamma = ABS_\gamma(S_n) & \textit{when } \gamma > 0,\\ = (n-1) & \textit{when } \gamma = 0,\\ > (n-1)\left(\dfrac{n-2}{n}\right)^\gamma = ABS_\gamma(S_n) & \textit{when } \gamma < 0. \end{cases}$$

Proof. For $\gamma = 0$, the result is trivial. Because the proofs of the desired inequalities for $\gamma > 0$ and $\gamma < 0$ are very similar to each other, we prove the inequality only for $\gamma > 0$. Thereby, in the rest of the proof, we suppose that $\gamma > 0$. The constraints $G \neq S_n$ and $n \geq 4$ guarantee that G has an edge xy such that $\min\{d_x, d_y\} \geq 2$. Assume that $d_x \geq d_y$. Take $N_G(y) = \{y_1, y_2, \ldots, y_r, x\}$ and $N_G(x) = \{x_1, x_2, \ldots, x_s, y\}$. Generate a graph $G^\star$ from G by dropping out the edges $y_1y, y_2y, \cdots, y_ry$ and by inserting $x_1y, x_2y, \cdots, x_ry$. By using Theorem 2, one obtains $ABS_\gamma(G) < ABS_\gamma(G^\star)$. If $G^\star = S_n$ then we are finished. If $G^\star \neq S_n$, then $G^\star$ contains an edge $x'y'$ such that $d_{x'} \geq d_{y'} \geq 2$, and hence, we apply the above transformation on all the neighbors of y', except x, of $G^\star$ to obtain another graph $G^{\star\star}$ satisfying $ABS_\gamma(G) < ABS_\gamma(G^\star) < ABS_\gamma(G^{\star\star})$. If $G^{\star\star} = S_n$, then we are finished. If $G^{\star\star} \neq S_n$, then we repeat this process (of applying the above graph transformation) until we obtain S_n. □

Lemma 4 ([24]). *If G is an n-vertex graph, then at most, two of the following properties can hold:*

(i). *The graph G is triangle free.*

(ii). *The minimum degree of G is more than $\frac{2n}{5}$.*

(iii). *The chromatic number of G is at least 3.*

The set of all different members of the degree sequence of a graph G is referred to as the degree set of G.

Theorem 4. *If G is a triangle-free graph, containing no component isomorphic to K_2, with $m \geq 2$ edges and n vertices, then*

$$ABS_\gamma(G)\begin{cases} \leq m\left(\dfrac{n-2}{n}\right)^\gamma & \textit{if } \gamma > 0,\\ \geq m\left(\dfrac{n-2}{n}\right)^\gamma & \textit{if } \gamma < 0. \end{cases}$$

In either case, the equality holds if and only if G is a completely bipartite graph.

Proof. Note that the function ψ defined as follows is strictly decreasing for $\gamma < 0$ and strictly increasing for $\gamma > 0$:

$$\psi(\alpha) = \left(\frac{\alpha - 2}{\alpha}\right)^{\gamma}, \quad \alpha > 2.$$

The definition of G implies that for every edge $xy \in E(G)$, the inequality $d_x + d_y \leq n$ holds, and hence

$$\psi(d_x + d_y) \begin{cases} \leq \psi(n) & \text{if} \quad \gamma > 0, \\ \geq \psi(n) & \text{if} \quad \gamma < 0, \end{cases}$$

with equality holds, in either case, if and only if $d_x + d_y = n$. Consequently, we have

$$ABS_{\gamma}(G) \begin{cases} \leq m\left(\dfrac{n-2}{n}\right)^{\gamma} & \text{if} \quad \gamma > 0, \\ \geq m\left(\dfrac{n-2}{n}\right)^{\gamma} & \text{if} \quad \gamma < 0. \end{cases}$$

with equality if and only if the equation $d_x + d_y = n$ holds for every edge $xy \in E(G)$.

It remains to be shown that G (being a triangle-free graph) is completely bipartite if and only if the equation $d_x + d_y = n$ holds for every edge $xy \in E(G)$. If G is completely bipartite, then the desired conclusion follows from the definition of G. Conversely, assume that the equation $d_x + d_y = n$ holds for every edge $xy \in E(G)$. Take $uv, vw \in E(G)$. Then, $d_u + d_v = n = d_v + d_w$, which gives $d_u = d_w$. Thus, the degree set of G has at most two elements. (Under the given constraint, if the degree set of G has two elements then adjacent vertices of G have different degrees.)

Next, we claim that G (being a triangle-free graph) is bipartite. Contrarily, assume that G is not bipartite. The graph G then contains a cycle of odd length (of at least 5), which implies that G is regular; otherwise, adjacent vertices of G have different degrees, which is not possible because of the existence of a cycle of odd length in G. Since $d_x + d_y = n$ for every edge $xy \in E(G)$, the graph must be $\frac{n}{2}$-regular, and n must be even. Since $\frac{n}{2} > \frac{2n}{5}$ and the chromatic number of G is greater than 2 (because we have contrarily assumed that G having at least one edge is not bipartite), we arrive at a contradiction to Lemma 4. Thus, G must be bipartite.

Let (A_1, A_2) be the bipartition of G. Take $a_1a_2 \in E(G)$ with $a_1 \in A_1$ and $a_2 \in A_2$. Then, a_1 must be adjacent to all vertices of A_2, and a_2 must be adjacent to all vertices of A_1 because $d_x + dy = n$ for every $xy \in E(G)$. Therefore, G is completely bipartite. □

We remark here that the part of Theorem 3 regarding $\gamma < 0$ follows from Theorem 4. Next, we give another consequence of Theorem 4.

Corollary 3. *If G is a triangle-free graph, containing no component isomorphic to K_2, with n vertices and with at least two edges, then*

$$ABS_{\gamma}(G) \leq \left\lfloor \frac{n^2}{4} \right\rfloor \left(\frac{n-2}{n}\right)^{\gamma}, \quad \textit{for } \gamma > 0;$$

where $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ is the only graph for which the equality sign in this inequality holds.

Proof. The well-known Turán Theorem guaranties $|E(G)| \leq \lfloor n^2/4 \rfloor$, where $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ is the only graph for which the equality sign in this inequality holds. Now, the required conclusion follows from Theorem 4. □

Since bipartite graphs are also triangle free, Corollary 4 implies the next result.

Corollary 4. *If G is a bipartite graph, containing no component isomorphic to K_2, with n vertices and with at least two edges, then*

$$ABS_\gamma(G) \leq \left\lfloor \frac{n^2}{4} \right\rfloor \left(\frac{n-2}{n}\right)^\gamma, \quad \text{for } \gamma > 0,$$

where $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ is the only graph for which the equality sign in this inequality holds.

Theorem 5. *If G is a graph, containing no component isomorphic to K_2, with $m \geq 2$ edges, then*

$$ABS_\gamma(G) \begin{cases} \leq m\left(\frac{m-1}{m+1}\right)^\gamma & \text{if } \gamma > 0, \\ \geq m\left(\frac{m-1}{m+1}\right)^\gamma & \text{if } \gamma < 0. \end{cases}$$

The equality holds, in either case, if and only if G is the star graph.

Proof. Note that the function ψ defined as follows is strictly decreasing for $\gamma < 0$ and strictly increasing for $\gamma > 0$:

$$\psi(\alpha) = \left(\frac{\alpha-2}{\alpha}\right)^\gamma, \quad \alpha > 2.$$

Note that the inequality $d_x + d_y \leq m + 1$ holds for every edge $xy \in E(G)$, and hence

$$\psi(d_x + d_y) \begin{cases} \leq \psi(m+1) & \text{when } \gamma > 0, \\ \geq \psi(m+1) & \text{when } \gamma < 0, \end{cases}$$

with equality, in either case, if and only if $d_x + d_y = m + 1$. Consequently, we have

$$ABS_\gamma(G) \begin{cases} \leq m \cdot \psi(m+1) & \text{when } \gamma > 0, \\ \geq m \cdot \psi(m+1) & \text{when } \gamma < 0. \end{cases}$$

with equality, in either case, if and only if $d_x + d_y = m + 1$ for every edge $xy \in E(G)$; that is, every edge of G is adjacent with all other edges of G. □

Theorem 3 confirms that S_n is the only graph with the least value of ABS_γ over the family of all n-vertex tree graphs for $\gamma < 0$. Next, by utilizing Theorem 5, we prove a result similar to this statement for connected graphs when $-\frac{3}{4} < \gamma < 0$.

Corollary 5. *For an n-vertex connected graph $G \neq S_n$, with $n \geq 3$, the following inequality holds*

$$ABS_\gamma(G) > (n-1)\left(\frac{n-2}{n}\right)^\gamma \quad \text{when } -\frac{3}{4} < \gamma < 0.$$

Proof. Assume that G has m edges. Since $m \geq 2$ and $G \neq S_n$, by using Theorem 5, we have

$$ABS_\gamma(G) > m\left(\frac{m-1}{m+1}\right)^\gamma \quad \text{for } -\frac{3}{4} < \gamma < 0. \tag{10}$$

Consider the function ϕ_γ defined as follows:

$$\phi_\gamma(\alpha) = \alpha\left(\frac{\alpha-1}{\alpha+1}\right)^\gamma, \quad \alpha \geq 2,$$

where γ is a fixed number satisfying $-\frac{3}{4} < \gamma < 0$. The derivative function ϕ'_γ of ϕ_γ is found as

$$\phi'_\gamma(\alpha) = \left(\frac{\alpha-1}{\alpha+1}\right)^\gamma \left(\frac{\alpha^2+2\gamma\alpha-1}{\alpha^2-1}\right).$$

Since $\alpha \geq 2$ and $-\frac{3}{4} < \gamma < 0$, the inequality $\phi'_\gamma(\alpha) > 0$ holds whenever $\alpha^2 + 2\gamma\alpha - 1 > 0$, which holds whenever

$$2\gamma > \frac{1}{\alpha} - \alpha \geq \frac{1}{2} - 2,$$

which is certainly true because $\alpha \geq 2$ and $-\frac{3}{4} < \gamma < 0$. Thus, $\phi'_\gamma(\alpha) > 0$, and hence, $\phi_\gamma(m) \geq \phi_\gamma(n-1)$, which together with (10) yield

$$ABS_\gamma(G) > (n-1)\left(\frac{n-2}{n}\right)^\gamma \quad \text{for} \quad -\frac{3}{4} < \gamma < 0.$$

□

5. Conclusions

We investigated the significance of the general ABS index ABS_γ on the data set of twenty-five benzenoid hydrocarbons for predicting their enthalpy of formation for $-10 \leq \gamma \leq 10$ and found that its predictive ability for the selected property of the considered hydrocarbons is comparable to other existing general indices of this type. We also proved the inequality $ABS_\gamma(G + rs) > ABS_\gamma(G)$ for $\gamma \geq 0$ whenever r and s are non-adjacent vertices in a graph G. Finally, we proved a number of extremal results regarding trees, general graphs, and triangle-free graphs of a given number of vertices. It would be interesting to examine the index ABS_γ on other data sets of chemical compounds for predicting their physicochemical properties. Another direction for possible future work regarding ABS_γ is the study of the behavior of this index of a non-complete graph G when a new edge is added to G and $\gamma < 0$.

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