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Research Article

On the $\mathcal{ABS}$ spectrum and energy of graphs

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Abstract: Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ be the eigenvalues of $\mathcal{ABS}$ matrix. In this paper, we characterize connected graphs with $\mathcal{ABS}$ eigenvalue $\eta_n > -1$. As a result, we determine all connected graphs with exactly two distinct $\mathcal{ABS}$ eigenvalues. We show that a connected bipartite graph has three distinct $\mathcal{ABS}$ eigenvalues if and only if it is a complete bipartite graph. Furthermore, we present some bounds for the $\mathcal{ABS}$ spectral radius (resp. $\mathcal{ABS}$ energy) and characterize extremal graphs. Also, we obtain a relation between $\mathcal{ABC}$ energy and $\mathcal{ABS}$ energy. Finally, the chemical importance of $\mathcal{ABS}$ energy is investigated and it shown that the $\mathcal{ABS}$ energy is useful in predicting certain properties of molecules.

Keywords: $\mathcal{ABS}$ matrix, spectral radius, $\mathcal{ABS}$ energy, QSPR analysis.

AMS Subject classification: 05C50, 05C09, 05C35, 05C92

1. Introduction

Throughout this article, we assume that G is a graph with vertex set $V(G)$ and edge set $E(G)$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $|E(G)| = m$. If two vertices v_i and v_j are adjacent, then we write it as $v_i \sim v_j$. We denote the degree of the vertex v_i by $d(v_i)$ (d_i for short). As usual, the complete graph, path graph and complete bipartite graph on n vertices are denoted by K_n, P_n and K_{n_1,n_2} $(n_1 + n_2 = n)$, respectively. Adjacency matrix of G is one of the well-studied graph matrix, denoted by $A(G)$ and defined as $A(G) = [a_{ij}]_{n\times n}$, where $a_{ij} = 1$ if and only if $v_i \sim v_j$ or 0, otherwise.

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If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $A(G)$, then the sum $\sum_{i=1}^{n} |\lambda_i|$ is called the energy of graph G and is denoted by $\mathcal{E}(G)$. The concept of graph energy, introduced by Gutman in 1978, slowly attracted mathematicians and chemists. In recent years, extensive research on graph energy has been carried out. For recent research on graph energy, see [1, 2, 9, 13, 14, 26] and refer to the book "Graph Energy" by Li, Shi, and Gutman [19]. The study of graph energy is extended to various graph matrices, including (signless) Laplacian matrix, distance matrix, degree-based graph matrices and distance-based graph matrices. More than 50 graph energies have been defined so far. See [17] for more details.

A topological index is a numerical quantity derived from the graph's structure. In literature, plenty of topological indices are defined and used as molecular descriptors (see [3, 12, 15, 16]). Most of the degree-based topological indices can be represented as $TI(G) = \sum_{v_i \sim v_j} \mathcal{F}(d_i, d_j)$, where $\mathcal{F}(d_i, d_j) = \mathcal{F}(d_j, d_i)$. As examples, we have first Zagreb index $\mathcal{F}(d_i, d_j) = d_i + d_j$, second Zagreb index $\mathcal{F}(d_i, d_j) = d_i d_j$, Randić index $(R(G))$ $\mathcal{F}(d_i, d_j) = \frac{1}{\sqrt{d_i d_j}}$, harmonic index $(H(G))$ $\mathcal{F}(d_i, d_j) = \frac{2}{d_i + d_j}$, sum-connectivity index $(\chi(G))$ $\mathcal{F}(d_i, d_j) = \frac{1}{\sqrt{d_i + d_j}}$, atom-bond connectivity index $(ABC(G))$ $\mathcal{F}(d_i, d_j) = \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$, atom-bond sum-connectivity index $(ABS(G))$ $\mathcal{F}(d_i, d_j) = \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}$, etc. For a topological index $TI(G)$, Das et al. [10] defined a general extended adjacency matrix as $\mathcal{T} = (t_{ij})_{n \times n}$, where $t_{ij} = \mathcal{F}(d_i, d_j)$ if $v_i \sim v_j$ or 0, otherwise. The sum of absolute values of all the eigenvalues of the matrix $\mathcal{T}$ is called the energy of the general extended adjacency matrix $\mathcal{T}$. In [10], Das et al. obtained several lower and upper bounds for the energy of the matrix $\mathcal{T}$, and deduced several known results about degree-based energies of graphs.

The ABS index was introduced recently by Ali et al. in [4]. It combines both sum-connectivity index and atom-bond sum connectivity index. Bounds on ABS index for the classes of (molecular) trees and general graphs are obtained in [4] and also extremal graphs are classified. Chemical applicability of ABS-index is demonstrated in [6, 25]. For more details about ABS index we refer to the survey article [5] by Ali et al. The $\mathcal{ABS}$ matrix of G is defined to be the matrix $\mathcal{ABS}(G) = (w_{ij})_{n \times n}$, where $w_{ij} = \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}$ if $v_i \sim v_j$ and 0, otherwise. We denote the eigenvalues of $\mathcal{ABS}(G)$ by $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$. The sum $\sum_{i=1}^{n} |\eta_i|$ is called the $\mathcal{ABS}$ energy of G and is denoted by $\mathcal{E}_{\mathcal{ABS}}(G)$. The study of properties of $\mathcal{ABS}$ matrix began recently. In [21], it is proved that the $\mathcal{ABS}$ Estrada index $(\sum_{i=1}^{n} e^{\eta_i})$ of trees is maximum from the star graph and it is minimum for the path graph. Also, in [20], the authors proved that $\mathcal{ABS}$ spectral radius of a tree is maximum for star graph and it is minimum for the path graph. The chemical importance of the $\mathcal{ABS}$ Estrada index and the $\mathcal{ABS}$

spectral radius are investigated separately in [20, 21], and it is shown that the $\mathcal{ABS}$ Estrada index and $\mathcal{ABS}$ spectral radius can be useful in predicting certain properties of molecules.

Motivated by this, in Section 2 of the paper, we characterize connected graphs with $\mathcal{ABS}$ eigenvalue $\eta_n > -1$. As a result, we determine all connected graphs with exactly two distinct $\mathcal{ABS}$ eigenvalues. Further, we show that a connected bipartite graph has three distinct $\mathcal{ABS}$ eigenvalues if and only if it is a complete bipartite graph. In Sections 3 and 4, we present some bounds for the $\mathcal{ABS}$ spectral radius (resp. $\mathcal{ABS}$ energy) and characterize extremal graphs. Also, we obtain a relation between $\mathcal{ABC}$ energy and $\mathcal{ABS}$ energy. In Section 5, the chemical importance of $\mathcal{ABS}$ energy is investigated and it shown that the $\mathcal{ABS}$ energy is useful to predict the boiling point and pi-electron energy of benzenoid hydrocarbons.

2. Properties of $\mathcal{ABS}$ eigenvalues

The following proposition is one of the basic properties of $\mathcal{ABS}$ eigenvalues. We omit its proof as it is straightforward.

Proposition 1. *Let G be a graph on n vertices. Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ be its $\mathcal{ABS}$-eigenvalues. Then $\sum_{i=1}^{n} \eta_i = 0$, $\sum_{i=1}^{n} \eta_i^2 = 2(m - H(G))$ and $\sum_{1\leq i<j\leq n} \eta_i\eta_j = H(G) - m$.*

Let M be a Hermitian matrix of order n. We denote the eigenvalues of M by $\theta_1(M) \geq \theta_2(M) \geq \cdots \geq \theta_n(M)$. The following lemma is the well-known Cauchy's interlacing theorem.

Lemma 1. [18] *Let M be a symmetric matrix of order n and let M_k be its leading principal $k \times k$ submatrix. Then $\theta_{n-k+i}(M) \leq \theta_i(M_k) \leq \theta_i(M)$ for $i = 1, 2, \ldots, k$.*

Theorem 1. *Let G be a graph on n vertices. Then the $\mathcal{ABS}$ eigenvalues of G are all equal if and only if $G \cong pK_2 \cup qK_1$, where $2p + q = n$.*

Proof. Suppose that the $\mathcal{ABS}$ eigenvalues of G are all equal. Then by Proposition 1, $\sum_{i}^{n} \eta_i = 0$, and so the $\mathcal{ABS}$ eigenvalues of G are zeros. Let H be a component of G. If $|V(H)| \geq 3$, then there exists a vertex x in H of degree at least two. Let y be a vertex of H adjacent to x. Then the principal minor of $\mathcal{ABS}(G)$ corresponding to the vertices x and y is non-zero. Thus, by Cauchy's interlacing theorem (see Lemma 1), the least eigenvalue of $\mathcal{ABS}(G)$ is non-zero, a contradiction. Hence, $|V(H)| \leq 2$. Therefore, $G \cong pK_2 \cup qK_1$, where $2p + q = n$. Conversely, if $G \cong pK_2 \cup qK_1$, then all the entries of $\mathcal{ABS}(G)$ are zeros. Thus, $\eta_1 = \eta_2 = \cdots = \eta_n = 0$. $\square$

The diameter of a graph G is the maximum distance between any pair of vertices in G and it is denoted by $diam(G)$. In the following theorem, we characterize connected graphs with $\eta_n(G) > -1$.

Theorem 2. *Let G be connected graph on n vertices. Then $\eta_n(G) > -1$ if and only if $G \cong K_n$ or P_3.*

Proof. Assume that $diam(G) \geq 2$ and $G \ncong P_3$. Let $x - y - z$ be an induced path in G. Then either $d(y) \geq 3$, $d(x) \geq 2$ or $d(z) \geq 2$. Let $\mathcal{ABS}[p, q, r]$ denote the principal submatrix of $\mathcal{ABS}(G)$ corresponding to the vertices p, q and r, where $p - q - r$ is an induced path in G. Let $\theta_1[p - q - r] \geq \theta_2[p - q - r] \geq \theta_3[p - q - r]$ be the eigenvalues of $\mathcal{ABS}[p, q, r]$. Then

$$\begin{aligned}
\theta_1[p-q-r] &= \sqrt{2}\,\sqrt{1 - \frac{1}{d(q)+d(r)} - \frac{1}{d(q)+d(p)}};\\
\theta_2[p-q-r] &= 0;\\
\theta_3[p-q-r] &= -\sqrt{2}\,\sqrt{1 - \frac{1}{d(q)+d(r)} - \frac{1}{d(q)+d(p)}}.
\end{aligned}$$

Also, by Cauchy's interlacing theorem (see Lemma 1), $\eta_n(G) \leq \theta_3[p - q - r]$.

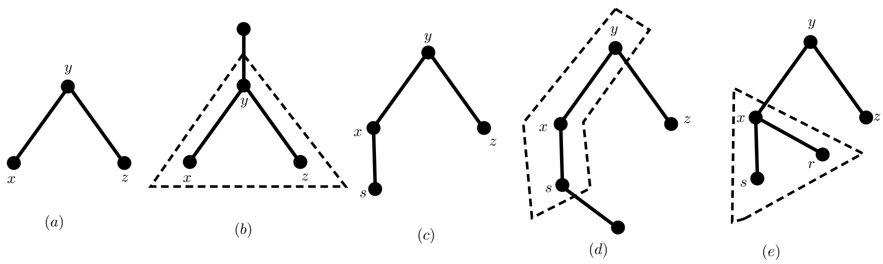

Figure 1. **Graphs considered in the proof of Theorem 2.**

Case 1: Let $d(y) \geq 3$, $d(x) \geq 1$ and $d(z) \geq 1$ (see Fig. 1(b)). Then
$2\left(1 - \dfrac{1}{d(y)+d(z)} - \dfrac{1}{d(y)+d(x)}\right) \geq 1$. Thus, $\eta_n(G) \leq \theta_3[x - y - z] \leq -1$.

Case 2: Let $d(y) = 2$, $d(x) \geq 2$ and $d(z) \geq 1$. If $d(z) \geq 2$, then
$2\left(1 - \dfrac{1}{d(y)+d(z)} - \dfrac{1}{d(y)+d(x)}\right) \geq 1$. So, $\eta_n(G) \leq \theta_3[x - y - z] \leq -1$. Otherwise, $d(z) = 1$. Let s be a vertex adjacent with the vertex x in G (see Fig. 1(c)). If $G \cong P_4$, then $\eta_n(G) = -1.0306 < -1$. Suppose $G \ncong P_4$, then either $d(x) \geq 3$ or $d(s) \geq 2$.

Subcase 2.1: Let $d(x) \geq 2$ and $d(s) \geq 2$ (see Fig. 1(d)). Then

$2\left(1-\dfrac{1}{d(s)+d(x)}-\dfrac{1}{d(y)+d(x)}\right)\geq 1$. Thus, $\eta_n(G)\leq\theta_3[s-x-y]\leq -1$.

Subcase 2.2: Let $d(x)\geq 3$ and $d(s)=1$. Then there exists a vertex r adjacent with the vertex x in G (see Fig. 1(e)).Therefore, $2\left(1-\dfrac{1}{d(s)+d(x)}-\dfrac{1}{d(r)+d(x)}\right)\geq 1$. Thus, $\eta_n(G)\leq\theta_3[s-x-r]\leq -1$.

Thus for a connected graph $G\ncong P_3$ with $diam(G)\geq 2$, $\eta_n(G)\leq -1$. Hence $G\cong K_n$ or P_3. Conversely, $\eta_n(K_n)=-\sqrt{\dfrac{n-2}{n-1}}>-1$ and $\eta_3(P_3)=-0.81649>-1$. This completes the proof of the theorem. $\square$

Corollary 1. *Let G be a connected graph of order $n\geq 2$. Then $\eta_n=-\sqrt{\dfrac{n-2}{n-1}}$ if and only if $G\cong K_n$.*

Proof. Suppose $\eta_n=-\sqrt{\dfrac{n-2}{n-1}}$. Then by Theorem 2, $G\cong K_n$ or P_3. Since $n_3(P_3)=-\sqrt{\dfrac{2}{3}}\left(\neq-\sqrt{\dfrac{1}{2}}\right)$, $G\cong K_n$. The converse part is direct. $\square$

Let B_1 and B_2 be two real matrices of same order, we write $B_1\preceq B_2$ if every entry in B_1 does not exceed the counterpart in B_2. The following lemma is useful to prove our next result.

Lemma 2. [18] *Let B_1, B_2 be non-negative matrices of order n. If $B_1\preceq B_2$, then $\rho(B_1)\leq\rho(B_2)$. Further, if B_1 is irreducible and $B_1\neq B_2$, then $\rho(B_1)<\rho(B_2)$.*

Theorem 3. *Let G be a connected graph of order $n>2$. Then $\mathcal{ABS}(G)$ has exactly two distinct eigenvalues if and only if $G\cong K_n$.*

Proof. Suppose G has exactly two distinct eigenvalues. Since G is a connected graph of order $n>2$, the matrix $\mathcal{ABS}(G)$ is irreducible, and thus by Perron-Frobenius theory its largest eigenvalue, i.e., $\eta_1(G)$ is a simple eigenvalue of G. So, $\eta_1(G)$ and $\eta_n(G)$ are the two distinct eigenvalues of G, and $\eta_2(G)=\eta_3(G)=\cdots=\eta_n(G)$. Let $B=\sqrt{\dfrac{n-2}{n-1}}A(K_n)$. Then the eigenvalues of B are $(n-1)\sqrt{\dfrac{n-2}{n-1}},\underbrace{-\sqrt{\dfrac{n-2}{n-1}},\ldots,-\sqrt{\dfrac{n-2}{n-1}}}_{n-1}$. Since $\mathcal{ABS}(G)\preceq B$, $\eta_1(G)\leq(n-1)\sqrt{\dfrac{n-2}{n-1}}$ by Lemma 2. Therefore, $-(n-1)\eta_n(G)\leq(n-1)\sqrt{\dfrac{n-2}{n-1}}$. That is, $\eta_n(G)\geq-\sqrt{\dfrac{n-2}{n-1}}>-1$. Hence by Theorem 2, $G\cong K_n$ or P_3. So, $G\cong K_n$ because P_3 has three distinct eigenvalues. The converse part is straightforward. $\square$

The following lemma is important to prove our next result.

Lemma 3. [18] *Let $C \in M_{n,m}$, $q = min\{n, m\}$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_q$ be the ordered singular values of C, and define the Hermitian matrix $\mathcal{H} = \begin{bmatrix} 0 & C \\ C^* & 0 \end{bmatrix}$. The ordered eigenvalues of $\mathcal{H}$ are $-\sigma_1 \leq \cdots \leq -\sigma_q \leq 0 = \cdots = 0 \leq \sigma_q \leq \cdots \leq \sigma_1$.*

Theorem 4. *Let G be a graph of order n. Let $M = (m_{ij})_{n\times n}$ be a non-negative symmetric matrix of order n, where m_{ij} is positive if and only if $v_i \sim v_j$. Then the graph G is bipartite if and only if the eigenvalues of the matrix M are symmetric about origin.*

Proof. Suppose G is a bipartite graph. Then the matrix M can be written as $M = \begin{bmatrix} 0 & C \\ C^T & 0 \end{bmatrix}$, where C is a rectangular matrix with non-negative entries. Therefore, by Lemma 3, the eigenvalues of M are symmetric about the origin.
Conversely, suppose the eigenvalues of M are symmetric about the origin. Then $trace(M^k) = 0$ for all odd integer $k > 0$. By the definition of the matrix M, one can easily check that $trace(M^k(G)) > 0$ if and only if $trace(A^k(G)) > 0$. Now, assume that G contains an odd cycle of length k. Then $trace(A^k(G)) > 0$ (see [7, Proposition 1.3.1]). So, $trace(M^k) > 0$, a contradiction. Thus, G must be a bipartite graph. □

The following corollary is immediate from the above theorem.

Corollary 2. *A graph G is bipartite if and only if the eigenvalues of $\mathcal{ABS}(G)$ are symmetric about origin.*

Theorem 5. *A connected bipartite graph G of order $n > 2$ has three distinct $\mathcal{ABS}$ eigenvalues if and only if G is a complete bipartite graph.*

Proof. From Perron Frobenius theorem and by Corollary 2, $\eta_1(G) > 0$ and $\eta_n(G)$ are simple $\mathcal{ABS}$ eigenvalues of G. Suppose G has a non-zero $\mathcal{ABS}$ eigenvalue other than $\eta_1(G)$ and $\eta_n(G)$. Then by Corollary 2, G must have at least four distinct $\mathcal{ABS}$ eigenvalues. Thus, 0 is an $\mathcal{ABS}$ eigenvalue of G with multiplicity $n - 2$. Hence, $rank(\mathcal{ABS}(G)) = 2$. Let U and W be the vertex partition sets of G. Let $u \in U$ and $w \in W$. Since G is a connected bipartite graph, the rows corresponding to the vertices u and w are linearly independent. Further, since $rank(\mathcal{ABS}(G)) = 2$ and G is bipartite, the rows corresponding to the vertices belonging to U(respectively, W) are in the linear span of the row vector corresponding to the vertex u (respectively, w). Thus, the vertices in U (respectively, W) share the same vertex neighborhood set. Assume that $w \in W$ and $w \notin N(u)$. Then w is not adjacent with any vertices of U. Therefore, w is an isolated vertex of G, a contradiction because G is a connected graph of order at least 3. Thus, $N(u) = W$ and $N(w) = U$. Therefore, G is a complete bipartite graph.

Conversely, if G is the complete bipartite graph K_{n_1,n_2} of order $n = n_1 + n_2 (\geq 3)$, then $\mathcal{ABS}(G) = \sqrt{1 - \frac{2}{n_1+n_2}}A(G)$. Therefore the $\mathcal{ABS}$ eigenvalues of G are $\sqrt{n_1n_2\left(1 - \frac{2}{n_1+n_2}\right)}, \underbrace{0, 0, \ldots, 0}_{n-2}, -\sqrt{n_1n_2\left(1 - \frac{2}{n_1+n_2}\right)}$. Thus, G has exactly three distinct $\mathcal{ABS}$ eigenvalues. □

3. Bounds for the $\mathcal{ABS}$ spectral radius

In this section, we give some bounds for the largest $\mathcal{ABS}$ eigenvalue $\eta_1(G)$.

Lemma 4. *Let G be graph of order n with maximum degree Δ and minimum degree δ. Then the row sums of $\mathcal{ABS}(G)$ are equal if and only if G is a regular graph.*

Proof. Suppose the row sums of $\mathcal{ABS}(G)$ are equal . Let $u, v \in V(G)$ such that $d(u) = \delta$ and $d(v) = \Delta$. Then

$$\sum_{v_i : u \sim v_i} \sqrt{1 - \frac{2}{\delta + d_i}} = \sum_{v_j : v \sim v_j} \sqrt{1 - \frac{2}{\Delta + d_j}}. \tag{3.1}$$

If $\delta \neq \Delta$, then $\sum_{v_j : v \sim v_j} \sqrt{1 - \frac{2}{\Delta + d_j}} \geq \Delta\sqrt{1 - \frac{2}{\Delta + \delta}} > \sum_{v_i : u \sim v_i} \sqrt{1 - \frac{2}{\delta + d_i}}$, a contradiction to the equation (3.1). Thus, $\delta = \Delta$. i.e., G is a regular graph. The converse part is straightforward. □

The following theorem gives a lower bound for $\eta_1(G)$ in terms of order and the atom-bond sum connectivity index of graph G.

Theorem 6. *Let G be a graph of order n, minimum degree δ and maximum degree Δ. Then $\eta_1(G) \geq \frac{2ABS(G)}{n}$. Further, equality holds if and only if G is a regular graph.*

Proof. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a vector in $\mathbb{R}^n$. Then

$$x^T\mathcal{ABS}(G)x = 2\sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}x_ix_j.$$

Set $x = (1, 1, \ldots, 1)^T$. Then by Rayleigh's inequality, $\eta_1(G) \geq \frac{x^T\mathcal{ABS}(G)x}{x^Tx} = \frac{2ABS(G)}{n}$, and the equality holds if and only if $x = (1, 1, \ldots, 1)^T$ is an eigenvector of $\mathcal{ABS}(G)$ corresponding to the eigenvalue $\eta_1(G)$. Suppose $\eta_1(G) = \frac{2ABS(G)}{n}$. Then the row sums of $\mathcal{ABS}(G)$ are equal. Therefore, by Lemma 4, G is a regular graph. □

Next, we provide a lower and upper bound for $\eta_1(G)$ in terms of order, size and the harmonic index of graph G.

Theorem 7. *Let G be a graph of order n and size m with no isolated vertices. Then*

$$\sqrt{\frac{2\,(m-H(G))}{n}} \leq \eta_1(G) \leq \sqrt{\frac{2(n-1)}{n}\,(m-H(G))} \tag{3.2}$$

with equality holds if and only if n is even and $G \cong \frac{n}{2}K_2$.

Proof. By Proposition 1,

$$n\eta_1^2 \geq \sum_{i=1}^{n} \eta_i^2 = 2(m-H(G)). \tag{3.3}$$

Since $\sum\limits_{i=1}^{n} \eta_i = 0$, $\eta_1^2 = \left(\sum\limits_{i=2}^{n} \eta_i\right)^2$. Therefore by Cauchy-Schwarz inequality, $\eta_1^2 \leq (n-1)\sum\limits_{i=2}^{n} \eta_i^2$ and the equality holds if and only if $\eta_2 = \eta_3 = \cdots = \eta_n$. So,

$$n\eta_1^2 \leq 2(n-1)\,(m-H(G))\,. \tag{3.4}$$

Thus from equations (3.3) and (3.4) we get the desired inequality. Suppose n is even and $G \cong \frac{n}{2}K_2$. Then $\mathcal{ABS}(G)$ is the null matrix, and so $\eta_1 = \eta_2 = \cdots = \eta_n = 0$ and $H(G) = m$. Thus the equalities in (3.2) holds. Conversely, suppose the right equality holds. Then from equation (3.3), $\eta_1^2 = \eta_2^2 = \cdots = \eta_n^2$. This implies that G has at most two distinct $\mathcal{ABS}$ eigenvalue. Therefore, by Theorems 1 and 3, either $G \cong K_n$ $(n > 2)$ or n is even and $G \cong \frac{n}{2}K_2$. If $G \cong K_n$, then $\eta_1^2 \neq \eta_2^2$, a contradiction. Thus, $G \cong \frac{n}{2}K_2$ for an even integer n. Similarly, the left equality holds if and only if $G \cong \frac{n}{2}K_2$ for an even integer n. □

Theorem 8. *Let G be a graph of order n with minimum degree δ and maximum degree Δ. Then $\sqrt{\delta(\delta-1)} \leq \eta_1(G) \leq \sqrt{\Delta(\Delta-1)}$. Further, equality holds if and only if G is a regular graph.*

Proof. From [18, Theorem 8.1.22], $\min\limits_{1\leq i\leq n}\{R_i\} \leq \eta_1(G) \leq \max\limits_{1\leq i\leq n}\{R_i\}$, where R_i is the row sum of the ith row of $\mathcal{ABS}(G)$. Moreover, the equality on both sides holds if and only if all the row sums of $\mathcal{ABS}(G)$ are equal. Now,

$$\max_{1\leq i\leq n}\{R_i\} = \max_{1\leq i\leq n} \sum_{v_i : v_i \sim v_j} \sqrt{1-\frac{2}{d_i+d_j}} \leq \sqrt{\Delta(\Delta-1)},$$

where the equality holds if and only if one of the components of G is a Δ-regular graph, and

$$\min_{1\leq i\leq n}\{R_i\} = \min_{1\leq i\leq n}\sum_{v_i:v_i\sim v_j}\sqrt{1-\frac{2}{d_i+d_j}} \geq \sqrt{\delta(\delta-1)},$$

where the equality holds if and only if one of the components of G is a δ-regular graph. Now, by Lemma 4, the row sums of $\mathcal{ABS}(G)$ is a constant if and only if G is regular. Thus, $\sqrt{\delta(\delta-1)} \leq \eta_1(G) \leq \sqrt{\Delta(\Delta-1)}$ and the equality on both sides holds if and only if G is a regular graph. □

The sum connectivity matrix of a graph G is a general extended adjacency matrix with $\mathcal{F}(d_i,d_j) = \dfrac{1}{\sqrt{d_i+d_j}}$. It is denoted by $\mathcal{S}(G)$. In the following theorem, we give a relation between the spectral radius of $\mathcal{S}(G)$ $(\rho(\mathcal{S}(G)))$ and $\eta_1(G)$.

Theorem 9. *If G is a connected graph of order $n \geq 2$, then*

$$\rho(\mathcal{S}(G))\min_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2} \leq \eta_1(G) \leq \rho(\mathcal{S}(G))\max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}.$$

Further, equality on both sides holds if and only if G is a regular graph or semiregular graph.

Proof. The matrices $\mathcal{ABS}(G)$ and $\mathcal{S}(G)$ are non-negative and irreducible. Moreover,

$$\mathcal{S}(G)\min_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2} \preceq \mathcal{ABS}(G) \preceq \mathcal{S}(G)\max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}.$$

Thus, by Lemma 2,

$$\rho(\mathcal{S}(G))\min_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2} \leq \eta_1(G) \leq \rho(\mathcal{S}(G))\max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}.$$

Now we consider the equality case. Suppose $\eta_1(G) = \rho(\mathcal{S}(G))\max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}$. Then by Lemma 2, $\mathcal{ABS}(G) = \mathcal{S}(G)\max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}$. This implies that, for every edge v_iv_j in G, $\sqrt{d_i+d_j-2} = \max_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}$. Therefore, d_i+d_j is constant for any edge v_iv_j of G. Let u (resp. v) be a vertex in G with maximum degree Δ (resp. minimum degree δ). Let $u\sim u_1$ and $v\sim v_1$. Then $d(u)+d(u_1) \geq \Delta+\delta \geq d(v)+d(v_1)$. Hence, $d_i+d_j = \delta+\Delta$, for all $v_iv_j \in E(G)$. Now, suppose there exists a vertex w in G such that $d(w) \in (\delta,\ \Delta)$. Then G has a component whose vertex degrees are either $d(w)$ or $\Delta+\delta-d(w)$. Therefore, G is disconnected, a contradiction. Thus, G is Δ-regular or $(\delta,\ \Delta)$-semiregular graph. Similarly, if $\eta_1(G) = \rho(\mathcal{S}(G))\min_{v_iv_j\in E(G)}\sqrt{d_i+d_j-2}$, then G is Δ-regular or $(\delta,\ \Delta)$-semiregular graph. The converse part is straightforward. □

Theorem 10. *If G is a connected graph with maximum degree Δ and minimum degree δ, then $\frac{2\chi(G)}{n}\sqrt{2\delta-2} \leq \eta_1(G) \leq \sqrt{\frac{2(\Delta-1)(n-1)}{n}}\,R(G)$, where the equality on the left side holds only if G is regular and the equality on the right side holds only if G is a complete graph.*

Proof. From [28, Corollary 1], we have

$$\frac{2\chi(G)}{n} \leq \rho(\mathcal{S}(G)) \leq \sqrt{\frac{n-1}{n}R(G)}, \tag{3.5}$$

where the left side equality holds only if $\mathcal{S}(G)$ has equal row sums, and the right equality holds only if G is a complete graph. Therefore by Theorem 8, we get the desired result. □

4. Properties of Atom-bond sum-connectivity energy

In this section, we present some bounds on $\mathcal{E}_{\mathcal{ABS}}(G)$.

Theorem 11. *Let G be a graph with $n \geq 2$ vertices and m edges. Then*

(i) $\mathcal{E}_{\mathcal{ABS}}(G) \geq 2\sqrt{m - H(G)}$. Equality holds if and only if $G \cong pK_{n_1,n_2} \cup qK_2 \cup rK_1$, where $n_1 + n_2 > 2$, $p = 0$ or 1 and $p(n_1 + n_2) + 2q + r = n$.

(ii) $\mathcal{E}_{\mathcal{ABS}}(G) \leq \sqrt{2n(m - H(G))}$. Equality holds if and only if $G \cong pK_2 \cup qk_1$, where $2p + q = n$.

Proof. (i) From [10, Theorem 4], we have $\mathcal{E}_{\mathcal{ABS}}(G) \geq \sqrt{2trace(\mathcal{ABS}^2(G))}$ and the equality holds if and only if $\eta_1 = -\eta_n$ and $\eta_2 = \eta_3 = \cdots = \eta_{n-1} = 0$. Since $trace(\mathcal{ABS}^2(G)) = 2m - H(G)$, we get $\mathcal{E}_{\mathcal{ABS}}(G) \geq 2\sqrt{m - H(G)}$. Suppose $\eta_1 = -\eta_n$ and $\eta_2 = \eta_3 = \cdots = \eta_{n-1} = 0$. Then G is bipartite (see, Corollary 2). Also, if H is a component of G, then $\mathcal{ABS}(H)$ has either two or three distinct eigenvalues, or all its eigenvalues are equal to 0. Thus, from Theorems 5, we get $H \cong K_{n_1,n_2}$ with $n_1+n_2 > 2$, K_2 or K_1. Furthermore, if K_{n_1,n_2} $(n_1+n_2 > 2)$ is a component of G, then all other components of G are either K_2 or K_1. Otherwise $\eta_2 > 0$, a contradiction.

(ii) From[10, Corollary 2], we have $\mathcal{E}_{\mathcal{ABS}}(G) \leq \sqrt{n\,trace(\mathcal{ABS}^2(G))}$ and the equality holds if and only of $|\eta_1| = |\eta_2| = \cdots = |\eta_n|$. Therefore, $\mathcal{E}_{\mathcal{ABS}}(G) \leq \sqrt{2n\,(m - H(G))}$. Suppose $|\eta_1| = |\eta_2| = \cdots = |\eta_n|$. Then the eigenvalues of $\mathcal{ABS}(G)$ are all equal or it has exactly two distinct eigenvalues. So, by Theorems 1 and 3, each component of G is K_{n_1} for some positive integer n_1. Furthermore, $n_1 = 1$ or 2. Otherwise $\eta_1 > \eta_2$. This completes the proof. □

To prove our next upper bound on $\mathcal{E}_{\mathcal{ABS}}(G)$, we need the following lemma.

Lemma 5. *[8] A regular connected graph G is strongly regular if and only if it has three distinct eigenvalues.*

Theorem 12. *Let G be a graph of order n with m edges. If $m = H(G)$ or $2(m-H(G)) \geq n$, then $\mathcal{E}_{\mathcal{ABS}}(G) \leq \frac{2ABS(G)}{n}+\sqrt{(n-1)\left(2m-2H(G)-\frac{4(ABS(G))^2}{n^2}\right)}$. Further, equality holds if and only if $G \cong pK_2 \cup qK_1$, where $2p+q=n$, $G \cong K_n$ or G is a non-complete strongly k-regular graph with $\mathcal{ABS}$ eigenvalues $\sqrt{k(k-1)}$ and $\pm\sqrt{\frac{(n-k)(k-1)}{n-1}}$.*

Proof. Using Cauchy-Schwarz inequality,

$$\mathcal{E}_{\mathcal{ABS}}(G) = \sum_{i=1}^{n} |\eta_i| = \eta_1 + \sum_{i=2}^{n} |\eta_i| \leq \eta_1 + \sqrt{(n-1)(2m-2H(G)-\eta_1^2)},$$

where the equality holds if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_n|$. Let $g(x) = x + \sqrt{(n-1)(2m-2H(G)-x^2)}$. Then by first derivative test, the function g is decreasing for $\sqrt{\frac{2(m-H(G))}{n}} \leq x \leq \sqrt{2(m-H(G))}$. Now, $\frac{2ABS(G)}{n} = \frac{2}{n}\sum_{v_iv_j\in E(G)}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}} \geq \frac{2}{n}\sum_{v_iv_j\in E(G)}\frac{d_i+d_j-2}{d_i+d_j} = \frac{2(m-H(G))}{n} \geq \sqrt{\frac{2(m-H(G))}{n}}$ (because $2(m-H(G)) \geq n$). That is, $\frac{2ABS(G)}{n} \geq \sqrt{\frac{2(m-H(G))}{n}}$. Upon combining the above inequality with Theorem 6, we get

$$\sqrt{\frac{2(m-H(G))}{n}} \leq \frac{2ABS(G)}{n} \leq \eta_1 \leq \sqrt{2(m-H(G))}. \tag{4.1}$$

Therefore,

$$\mathcal{E}_{\mathcal{ABS}}(G) \leq g(\eta_1) \leq g\left(\frac{2ABS(G)}{n}\right) = \frac{2ABS(G)}{n}+\sqrt{(n-1)\left(2m-2H(G)-\frac{4(ABS(G))^2}{n^2}\right)}. \tag{4.2}$$

Suppose the equality in equation (4.2) holds. Then $\eta_1 = \frac{2ABS(G)}{n}$ and $|\eta_2| = |\eta_3| = \cdots = |\eta_n|$. Thus, $\mathcal{ABS}(G)$ has at most three distinct eigenvalues. If $\mathcal{ABS}(G)$ has at most two distinct eigenvalues, then by Theorems 1 and 3, $G \cong pK_2 \cup qK_1$, where $p+q=n$, or $G \cong K_n$. Otherwise, $\mathcal{ABS}(G)$ has exactly three distinct eigenvalues. Now, by Theorem 6, G is k-regular graph for some constant k, and so $\mathcal{ABS}(G) = \sqrt{\frac{k-1}{k}}A(G)$. If $\mathcal{ABS}(G)$ has exactly three distinct eigenvalues, then G has exactly three distinct eigenvalues. Therefore by Lemma 5, G must be a non-complete strongly regular graph. Conversely, if $G \cong pK_2 \cup qK_1$, where $2p+q=n$, or $G \cong K_n$, then one can easily see that the equality in (4.2) holds. Suppose G is a non-complete strongly

k-regular graph, then $\eta_1 = \sqrt{k(k-1)}$, $|\eta_j| = \sqrt{\dfrac{(n-k)(k-1)}{n-1}}$ for $j = 2, 3, \ldots, n$. Now, one can easily check that equality in (4.2) holds. This completes the proof of the theorem. □

The following lemmas are useful to prove our next result.

Lemma 6. [23] *If $M = (m_{ij})$ is a Hermitian $n \times n$ matrix, then* $|\theta_1(M) - \theta_n(M)| \geq 2 \max_j \left(\sum_{k:k\neq j} |m_{jk}|^2 \right)^{\frac{1}{2}}$.

Lemma 7. *Let G be a connected graph of order $n \geq 2$ with maximum degree Δ and minimum degree δ. Then*

$$2\sqrt{\frac{\Delta\,(\Delta+\delta-2)}{\Delta+\delta}} \leq \eta_1 + |\eta_n| \leq 2\sqrt{m - H(G)}.$$

Proof. By Lemma 6,

$$\eta_1 + |\eta_n| \geq 2 \max_i \left(\sum_{v_j : v_i \sim v_j} \frac{d_i + d_j - 2}{d_i + d_j} \right)^{1/2} \geq 2\sqrt{\frac{\Delta(\Delta+\delta-2)}{\Delta+\delta}}.$$

Proving the left inequality. Now, by Cauchy-Schwarz inequality and from Proposition 1,

$$\eta_1 + |\eta_n| \leq \sqrt{2(\eta_1^2 + \eta_n^2)} \leq \sqrt{4(m - H(G))} = 2\sqrt{m - H(G)}.$$

□

Theorem 13. *Let G be (n,m)-graph with maximum degree Δ. If $\dfrac{2\,(m - H(G))}{n} \leq \dfrac{\Delta\,(\Delta-1)}{\Delta+1}$, $\mathcal{E}_{\mathcal{ABS}}(G) \leq 2\sqrt{\dfrac{\Delta\,(\Delta-1)}{\Delta+1}} + \sqrt{2(n-2)\left(m - H(G) - \dfrac{\Delta\,(\Delta-1)}{\Delta+1}\right)}$. Equality holds if and only if $G \cong pK_{1,\Delta} \cup qK_2 \cup rK_1$, where $p = 0$ or 1 and $p(\Delta+1) + 2q + r = n$.*

Proof. Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ be the $\mathcal{ABS}$ eigenvalues of G. Using Cauchy-Schwarz inequality,

$$\mathcal{E}_{\mathcal{ABS}}(G) = \eta_1 + |\eta_n| + \sum_{i=2}^{n-1} |\eta_i| \leq \eta_1 + |\eta_n| + \sqrt{\sum_{i=2}^{n-1} (n-2)|\eta_i|^2},$$

where the equality holds if and only if $|\eta_2| = |\eta_3| = \cdots = |\eta_{n-1}|$. Therefore, by Proposition 1,

$$\mathcal{E}_{\mathcal{ABS}}(G) \leq \eta_1 + |\eta_n| + \sqrt{(n-2)(2m - 2H(G) - \eta_1^2 - \eta_n^2)}.$$

Further, by A.M.-G.M. inequality, $2\sqrt{\eta_1\eta_n} \leq \eta_1 + |\eta_n|$ and the equality holds if and only if $\eta_1 = |\eta_n|$, Thus

$$\mathcal{E}_{\mathcal{ABS}}(G) \leq \eta_1 + |\eta_n| + \sqrt{(n-2)\left(2m - 2H(G) - \frac{(\eta_1 + |\eta_n|)^2}{2}\right)}.$$

Let $f(x) = 2x + \sqrt{(n-2)(2m - 2H(G) - 2x^2)}$. Then f is decreasing for $\sqrt{\frac{2(m - H(G))}{n}} \leq x \leq \sqrt{m - H(G)}$. By Lemma 7,

$$\sqrt{\frac{2(m - H(G))}{n}} \leq \sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}} \leq \frac{\eta_1 + |\eta_n|}{2} \leq \sqrt{m - H(G)}.$$

So,

$$\begin{aligned} E_{\mathcal{ABS}}(G) &\leq f\left(\frac{\eta_1 + |\eta_n|}{2}\right) \leq f\left(\sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}}\right) \\ &= 2\sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}} + \sqrt{(n-2)\left(2m - 2H(G) - 2\frac{\Delta(\Delta-1)}{\Delta+1}\right)}. \end{aligned} \tag{4.3}$$

Suppose the equality in equation (4.3) holds. Then $\eta_1 = |\eta_n| = \sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}}$ and $|\eta_2| = |\eta_3| = \cdots = |\eta_{n-1}|$. Thus, by Perron-Frobenius theorem, G is a bipartite graph. If $\Delta = 1$, then, $G \cong qK_2 \cup rK_1$, where $2q + r = n$. Otherwise, $\Delta > 1$, and so $\eta_1 = |\eta_n| > 0$. Let H be component of G having a vertex of degree Δ. Since G is bipartite, $K_{1,\Delta}$ is an induced subgraph of H. So, by Cauchy's interlacing theorem, $\eta_1(H) \geq \eta_1(K_{1,\Delta}) = \sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}}$. Moreover the equality holds if and only if $H \cong K_{1,\Delta}$. Now, $\eta_1 = \sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}} \geq \eta_1(H)$ because H is a component of G. Therefore, $\eta_1(H) = \eta_1 = \frac{\Delta(\Delta-1)}{\Delta+1}$ and $H \cong K_{1,\Delta}$. Further, 0 is an $\mathcal{ABS}$ eigenvalue of H, and thus $\mathcal{ABS}$ eigenvalues of G are $\eta_1 = |\eta_n| = \sqrt{\frac{\Delta(\Delta-1)}{\Delta+1}}$ and $|\eta_2| = |\eta_3| = \cdots = |\eta_{n-1}| = 0$. Therefore, if $H_1 \ncong H$ is a component of G, then all its $\mathcal{ABS}$ eigenvalues are equal to 0. Therefore, by Theorem 1, $H_1 \cong K_2$ or K_1. Thus $G \cong pK_{1,\Delta} \cup qK_2 \cup rK_1$, where $p = 0$ or 1 and $p(\Delta+1) + 2q + r = n$. Conversely, if $G \cong pK_{1,\Delta} \cup qK_2 \cup rK_1$, where $p = 0$ or 1 and $p(\Delta+1) + 2q + r = n$, then one can easily verify that the equality holds. □

Theorem 14. *Let $\varphi_1 \geq \varphi_2 \geq \cdots \geq \varphi_n$ be the $\mathcal{ABC}$-eigenvalues and $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ be the $\mathcal{ABS}$ eigenvalues of a graph G without pendent vertices. Then $\mathcal{E}_{\mathcal{ABS}}(G) \geq \sqrt{\frac{2}{n}}\mathcal{E}_{\mathcal{ABC}}(G)$.*

Proof. We have,

$$
\begin{aligned}
(\mathcal{E}_{\mathcal{ABS}}(G))^2 &= \left(\sum_{i=1}^{n}|\eta_i|\right)^2 = \sum_{i=1}^{n}\eta_i^2 + 2\sum_{i<j}|\eta_i||\eta_j| \\
&\geq \sum_{i=1}^{n}\eta_i^2 + 2\left|\sum_{i<j}\eta_i\eta_j\right| \quad \text{(by triangle inequality)} \\
&= 2\sum_{i=1}^{n}\eta_i^2 \quad \left(\text{because} \sum_{i=1}^{n}\eta_i^2 = -2\sum_{i<j}\eta_i\eta_j\right) \\
&= 4\sum_{v_iv_j\in E(G)}\frac{d_i+d_j-2}{d_i+d_j} \\
&\geq 4\sum_{v_iv_j\in E(G)}\frac{d_i+d_j-2}{d_id_j} \\
&= 2\sum_{i=1}\varphi_i^2 \geq \frac{2}{n}\left(\sum_{i=1}|\varphi_i|\right)^2 \text{(by Cauchy-Schwarz inequality)} \\
&= \frac{2}{n}\left(\mathcal{E}_{\mathcal{ABC}}(G)\right)^2.
\end{aligned}
$$

Thus, $\mathcal{E}_{\mathcal{ABS}}(G) \geq \sqrt{\frac{2}{n}}\mathcal{E}_{\mathcal{ABC}}(G)$. □

5. QSPR analysis of benzenoid hydrocarbon

In this section, we show that the physicochemical properties, namely, the boiling point (BP) and pi-electron energy ($\mathcal{E}_\pi$)of benzenoid hydrocarbons can be modeled using $\mathcal{ABS}$-energy. The experimental values listed in this section are taken from [11, 24, 27]. The hydrogen-suppressed molecular graphs are depicted in Figure 2. The calculated values of $\mathcal{ABS}$ energy for benzenoid hydrocarbons are shown in Table 1 .

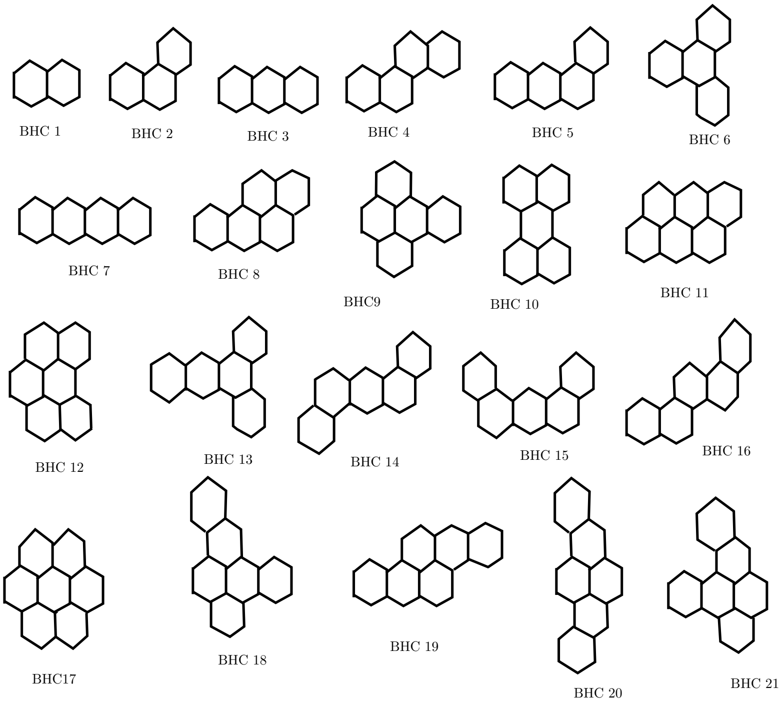

Figure 2. **Hydrogen-suppressed molecular graph of benzenoid hydrocarbons**

Compound	$\mathcal{E}_{\mathcal{ABS}}$	BP	$\mathcal{E}_{\pi}$
BHC1	10.089	218	13.6832
BHC2	14.5445	338	19.4483
BHC3	14.4865	340	19.3137
BHC4	18.9799	431	25.1922
BHC5	18.9015	425	25.1012
BHC6	19.0111	429	25.2745
BHC7	18.8744	440	24.9308
BHC8	21.5036	496	28.222
BHC9	21.5786	493	28.3361
BHC10	21.4939	497	28.2453
BHC11	24.0287	547	31.253

Compound	$\mathcal{E}_{\mathcal{ABS}}$	BP	$\mathcal{E}_{\pi}$
BHC12	23.5972	542	31.4251
BHC13	23.4346	535	30.9418
BHC14	23.4184	536	30.8805
BHC15	23.3769	531	30.8795
BHC16	23.4463	519	30.9432
BHC17	26.7119	590	34.5718
BHC18	25.9835	592	34.0646
BHC19	25.915	596	33.1892
BHC20	25.9357	594	33.9542
BHC21	25.9565	595	34.0307
-	-	-	-

Table 1. Experimental physicochemical properties and theoretical $\mathcal{ABS}$ energy of benzenoid hydrocarbons.

Consider the following model:

$$Y = A(\pm S_e)\mathcal{E}_{\mathcal{ABS}} + B(\pm S_e), \tag{5.1}$$

where Y, A, S_e and B denote the property, slope, standard error of coefficients and intercept, respectively. We denote the correlation coefficient, standard error of the

model, the F-test value and the significance by r, SE, F and SF, respectively.
For benzenoid hydrocarbons, it is found that the $\mathcal{ABS}$ energy has a strong correlation with the boiling point and pi-electron energy. In fact, we get the following regression equations for benzenoid hydrocarbons using model (5.1).

$$BP = 22.684(\pm 0.4013)\mathcal{E}_{\mathcal{ABS}} + 2.25(\pm 8.7952), \tag{5.2}$$

$$r^2 = 0.9941,\ SE = 7.8838,\ F = 3194.002,\ SF = 1.23 \times 10^{-22}.$$

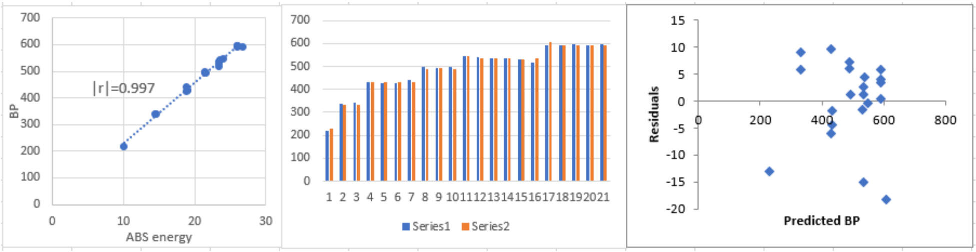

Figure 3. Linear relation of $\mathcal{ABS}$ energy with BP, experimental and predicted BP and residual plot.

$$\mathcal{E}_{\pi} = -1.2668(\pm 0.01235)\mathcal{E}_{\mathcal{ABS}} + 1.0586(\pm 0.2706), \tag{5.3}$$

$$r^2 = 0.9982,\ SE = 0.2425, F = 10522.29,\ SF = 1.54 \times 10^{-27}.$$

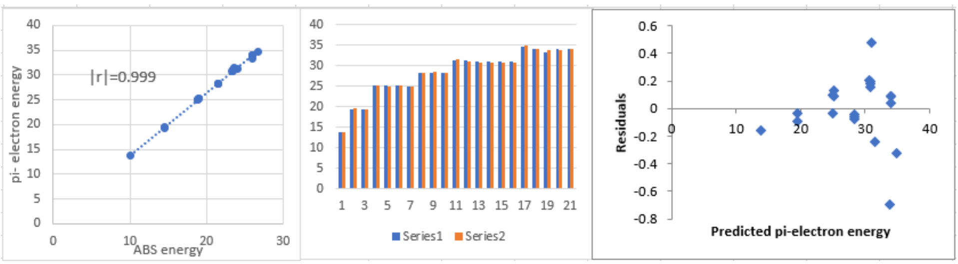

Figure 4. Linear relation of $\mathcal{ABS}$ energy with pi-electron energy, experimental and predicted pi-electron energy and residual plot.

The data variance for BP and pi-electron energy is around 99%. The standard errors are very low, particularly in model (5.3), where they are significantly small. This low standard error enhances the model's consistency and increases the F-value, especially for pi-electron energy. The SF values are significantly below 0.05. The predicted properties from model (5.1) are compared with the experimental properties using bar diagrams, where series 1 is related to experimental value and series 2 is related to predicted value. These figures show that the experimental and predicted data align

well. Additionally, the residuals are randomly scattered around the zero line, indicating that the model is consistent.
In [11, 22, 24, 25, 27] the QSPR analysis of benzenoid hydrocarbons is done using the second-degree based entropy, ve-degree irregularity index, Albertson index, first and second status connectivity indices, first and second eccentric connectivity indices, Wiener index, Sombor index, reduced Sombor index and ABS index. It is observed that the $|r|$ value obtained for BP using $\mathcal{E}_{\mathcal{ABS}}$ is better than that of $|r|$ value obtained from these indices. Further, $\mathcal{E}_{\mathcal{ABS}}$ have high pi-electron energy predictive ability compared to second-degree based entropy and ABS index. With the smaller standard error and higher F-value of the proposed models, we can conclude that the performance of the models is better than that of the models discussed in [25] using ABS index.

6. Conclusions

In this work, we have determined all connected graphs with $\eta_n > -1$. As a result, graphs with two distinct $\mathcal{ABS}$ eigenvalues are classified. Also, bipartite graphs with three distinct $\mathcal{ABS}$ eigenvalues are determined. Further, some bounds on the spectral radius and energy of the matrix $\mathcal{ABS}(G)$ are obtained. Also, the chemical importance of $\mathcal{ABS}$ energy is demonstrated. The problem of characterizing non-bipartite graphs with three distinct $\mathcal{ABS}$ eigenvalues remains open. As a future work, the problem of obtaining sharp bounds for the spectral radius and energy of the matrix $\mathcal{ABS}(G)$ in terms of graph parameters would be interesting.

Statements and Declarations

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