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Reduced Sombor Coindex of Graph Operations

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ABSTRACT: Here, we introduce a new parameter, called reduced Sombor coindex and we compute the results on reduced Sombor coindex for certain standard graphs. Also, we concerned to compute the Reduced Sombor coindex of certain graph operations like cartesian product, strong product, direct product, lexicographic product of two graphs. We also compute the bounds of the reduced Sombor coindex. The chemical applicability of this parameter is discussed by comparing it with the π-electron energy of some selected hetero molecules and by comparing it with the π-electron energy of some selected PAHs.

Keywords: Hetero molecules, PAHs, graph operations, reduced Sombor index, Sombor index, Sombor coindex, reduced Sombor coindex.

Contents

1. Introduction

Topological indices or molecular descriptors are mathematical formulae which can be applied to any graph and which play an important role in Mathematical Chemistry. Molecular descriptors have been used in the development of Quantitative Structure Activity Relationships (QSAR) and Quantitative Structure Property Relationships (QSPR). The topological index that depends on the degree of the vertices of the graph G, is known as the Vertex-degree-based index. Similarly, an edge-degree-based is also introduced. Numerous topological indices, including the Wiener index [5], Zagreb index [6], and others, have been examined in the QSAR/QSPR models. Out of all the molecular descriptors, the first and second Zagreb indices [6] are the most helpful. They are as follows

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

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The coindex of a graph is a topological index that measures the non-adjacency properties of vertices in a graph. Ashrafi *et al.* [1] defined the first Zagreb coindex and the second Zagreb coindex as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d(u) + d(v)],$$

and

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d(u)d(v),$$

Where $d(u)$ denotes the degree of u in G.
Gutman introduced a vertex degree based molecular discriptor called Sombor index [7] defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ denotes the degree of u in G.
In [4] reduced Sombor index is defined as

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$

where $d(u)$ denotes the degree of u in G.
Later Chinglensana *et al.*[12] defined a new topological index called Sombor coindex of graphs, defined as

$$\overline{SO}(G) = \sum_{uv \notin E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ denotes the degree of u in G.
In [2], Boregowda *et* al. Compared neighbors degree sum energy of graphs with the π-electron energy of some molecules containing hetero atoms and also with some selected polyaromatic hydrocarbons.
In [11], Narahari *et* al. Compared the π-electron energy of some molecules containing hetero atoms with the reverse Sombor energy of a graph .
In this paper, we consider simple, finite, connected and undirected graph $G = (V, E)$ with n vertices and m edges. We denote the vertex set of G by $V(G)$ and the edge set of G by $E(G)$ and $d(u), d(v)$ are the degrees of the vertices u and v in G. The degree of a vertex $d(u)$ is defined as the number of edges that are incident with the vertex u in G. Also, Δ and δ are maximum degree and minimum degree respectively. A simple graph $\overline{G}$ is the compliment of graph G. Two vertices u and v in G are adjacent, if and only if are not adjacent in $\overline{G}$. Hence, $(u, v) \in E(G)$ if and only if $(u, v) \notin E(\overline{G})$. And the number of edges in $\overline{G}$ denoted by $\overline{m}$ is defined as $\overline{m} = \begin{pmatrix} n \\ 2 \end{pmatrix} - m$. For any unexplained notations see [3]. We begin with the fundamental definitions which are essential.

2. Preliminaries

Definition 2.1 *The cartesian product [12] of G_1 and G_2, denoted by $G_1 \square G_2$ is a graph with vertex set $V(G_1 \square G_2) = V(G_1) \times V(G_2)$, where two vertices (u_i, v_j) and (u_k, v_l) are adjacent if and only if $u_i = u_k$ and $v_j \sim v_l \in E(G_2)$ or $u_i \sim u_k \in E(G_1)$ and $v_j = v_l$. In this graph $|E(G_1 \square G_2)| = n_1 m_2 + m_1 n_2$ where n_i and m_i denotes the number of vertices and edges respectively of G_i where $i = 1, 2$ and $d_{G_1 \square G_2}(u_i, v_j) = d_{G_1}(u_i) + d_{G_2}(v_j)$*

Definition 2.2 . *The composition (or Lexicographic product) [12] of G_1 and G_2, denoted by $G_1[G_2]$ is a graph with vertex set $V(G_1[G_2]) = V(G_1) \times V(G_2)$ in which any two vertices (u_i, v_j) and (u_k, v_l) are adjacent whenever $u_i \sim u_k$ in G_1 or $u_i = u_k$ and $v_j \sim v_l$ in G_2. In the graph $G_1[G_2], |V(G_1[G_2])| = n_1 n_2, |E(G_1[G_2])| = n_1 m_2 + m_1 n_2^2$ where n_i and m_i denotes the number of vertices and edges respectively of G_i where $i = 1, 2$ and $d_{G_1[G_2]}(u_i, v_j) = n_2 d_{G_1}(u_i) + d_{G_2}(v_j)$.*

Definition 2.3 . *The Direct product (or Tensor product) [8] of G_1 and G_2, denoted by $G_1 \otimes G_2$ is the graph with vertex set $V(G_1 \otimes G_2) = V(G_1) \times V(G_2)$ in which two vertices $(u_i, v_j) \sim (u_k, v_l)$ whenever $u_i \sim u_k$ in G_1 and $v_j \sim v_l$ in G_2. In this graph $|V(G_1 \otimes G_2)| = n_1n_2, |E(G_1 \otimes G_2)| = m_1m_2$ where n_i and m_i denotes the number of vertices and edges respectively of G_i where $i = 1, 2$ and $d_{G_1 \otimes G_2}(u_i, v_j) = d_{G_1}(u_i)d_{G_2}(v_j)$.*

Definition 2.4 . *The strong product [10] of G_1 and G_2, denoted by $G_1 \boxtimes G_2$ is the graph with vertex set $V(G_1 \boxtimes G_2) = V(G_1) \times V(G_2)$ in which two vertices $(u_i, v_j) \sim (u_k, v_l)$ if either ($u_i = u_k$ and $v_j \sim v_l$ in G_2) or ($u_i \sim u_k$ in G_1 and $v_j = v_l$) or ($u_i \sim u_k$ in G_1 and $v_i \sim v_l$ in G_2). In $G_1 \boxtimes G_2$, we have $|V(G_1 \boxtimes G_2)| = n_1n_2, |E(G_1 \boxtimes G_2)| = n_1m_2 + m_1n_2 + 2m_1m_2$ where n_i and m_i denotes the number of vertices and edges respectively of G_i where $i = 1, 2$ and $d_{G_1 \boxtimes G_2}(u_i, v_j) = d_{G_1}(u_i) + d_{G_2}(v_j) + d_{G_1}(u_i)d_{G_2}(v_j)$.*

3. Reduced Sombor Coindex of Graphs

We define a new topological index called reduced Sombor coindex of a graph, inspired by the Zagreb coindex [1], reduced Sombor [4] and the Sombor coindex [12] of graphs. The reduced Sombor coindex $\overline{RSO}(G)$ of a graph G, is defined as follows:

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u) - 1)^2 + (d(v) - 1)^2},$$

where $E(G)$ is the edge set of G and $d(u), d(v)$ denote the degrees of the vertices $u, v \in V(G)$ respectively.

Proposition 3.1 *(i) For C_n, $n \geq 4$, $\overline{C_n}$ has $[(n-3) + \sum_{k=1}^{n-3} k]$ number of $(2, 2)$ adjacent edges, therefore, by the definition of reduced Sombor coindex we have*

$$\begin{aligned}
\overline{RSO}(G) &= \sum_{uv \notin E(G)} \sqrt{(d(u) - 1)^2 + (d(v) - 1)^2} \\
\overline{RSO}(C_n) &= [(n-3) + \{1 + 2 + 3 + ... + (n-3)\}]\sqrt{(2-1)^2 + (2-1)^2} \\
&= \sqrt{2}[(n-3) + \sum_{k=1}^{n-3} k]
\end{aligned}$$

(ii) Let $K_{p,q}$, with $p, q \geq 2$, be a complete bipartite graph with $(p + q)$ vertices and pq edges. The compliment of $K_{p,q}$ has $\sum_{k=1}^{p-1} k$ number of (q, q) adjacent edges and $\sum_{k=1}^{q-1} k$ number of (p, p) adjacent edges. Hence by the definition of reduced Sombor coindex we have

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u) - 1)^2 + (d(v) - 1)^2}$$

$$\overline{RSO}(K_{p,q}) = \sqrt{2}(q-1)\sum_{k=1}^{p-1} k + \sqrt{2}(p-1)\sum_{k=1}^{q-1} k$$

$$\overline{RSO}(K_{p,q}) = \sqrt{2}[(q-1)\sum_{k=1}^{p-1} k + (p-1)\sum_{k=1}^{q-1} k]$$

(iii) For W_n, $n \geq 5$, $\overline{W_n}$ has $[(n-4) + \sum_{k=1}^{n-4} k]$ number of $(3, 3)$ adjacent edges.

By the definition of reduced Sombor coindex we have

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}$$
$$= 2\sqrt{2}(n-4) + 2\sqrt{2}\sum_{k=1}^{n-4} k$$
$$\overline{RSO}(W_n) = 2\sqrt{2}[(n-4) + \sum_{k=1}^{n-4} k].$$

(iv) For any path $P_n, n \geq 5$, $\overline{P_n}$ has only one $(1,1)$ adjacent edge , $(2n-6)$ number of $(1,2)$ adjacent edges and $\sum_{k=1}^{n-4} k$ number of $(2,2)$ adjacent edges and by the definition of reduced Sombor coindex we have

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}$$
$$\overline{RSO}(P_n) = (2n-6) + \sqrt{2}\sum_{k=1}^{n-4} k.$$

Notice that $\overline{RSO}(K_n) = 0$ because $\overline{K_n}$ is empty graph. Also, in Star graph $K_{1,n}$ degree of all n vertices is one . Hence $\overline{RSO}(K_{1,n}) = 0$

4. Results on Reduced Sombor Coindex of Graphs

Theorem 4.1 *If $P_{n_1} \square P_{n_2}$ is the cartesion product of two paths P_{n_1} and P_{n_2}, $n_1, n_2 \geq 3$, then*

$$\begin{aligned}\overline{RSO}(P_{n_1} \square P_{n_2}) =& 6\sqrt{2} + 8(n_1+n_2-5)\sqrt{5} + 4(n_1-2)(n_2-2)\sqrt{10} \\ &+ [4(n_1-2)(n_2-2) + (n_1-3)(2n_1-5) + (n_2-3)(2n_2-5) + 2]2\sqrt{2} \\ &+ [2(n_1+n_2-4)\{(n_1-3)(n_2-2) + (n_2-3)\}]\sqrt{13} \\ &+ [\frac{1}{2}(n_1-2)(n_2-3)(n_2-4) + \\ &\frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 + (n_1-3)(n_2-2)(n_2-3)]3\sqrt{2}.\end{aligned}$$

Proof: For the graphs P_{n_1} and P_{n_2}, $V(P_{n_1}) = \{u_1, u_2, u_3, \cdots, u_{n_1}\}$ and $V(P_{n_2}) = \{v_1, v_2, v_3, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and P_{n_2} respectively. Based on the degree of each vertex of the graph $P_{n_1} \square P_{n_2}$, we obtained the fallowing number of non-adjacent edges, as shown in the below table.

$(d(u), d(v))$	Number of non-adjacent edges
(2,2)	6
(2,3)	$8(n_1+n_2-5)$
(2,4)	$4(n_1-2)(n_2-2)$
(3,3)	$4(n_1-2)(n_2-2) + (n_1-3)(2n_1-5) + (n_2-3)(2n_2-5) + 2$
(3,4)	$2(n_1+n_2-4)[(n_1-3)(n_2-2) + (n_2-3)]$
(4,4)	$\frac{1}{2}(n_1-2)(n_2-3)(n_2-4) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 + (n_1-3)(n_2-2)(n_2-3)$

By the definition, we have

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}$$

$$\overline{RSO}(P_{n_1} \Box P_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l) \notin E(P_{n_1} \Box P_{n_2})} \sqrt{[(d_{P_{n_1}}(u_i) + d_{P_{n_2}}(v_j)) - 1]^2 + [(d_{P_{n_1}}(u_k) + d_{P_{n_2}}(v_l)) - 1]^2}$$

Using the above table, on simplification, we get

$$\begin{aligned}\overline{RSO}(P_{n_1} \Box P_{n_2}) =& 6\sqrt{2} + 8(n_1+n_2-5)\sqrt{5} + 4(n_1-2)(n_2-2)\sqrt{10} \\ &+ [4(n_1-2)(n_2-2) + (n_1-3)(2n_1-5) + (n_2-3)(2n_2-5) + 2]2\sqrt{2} \\ &+ [2(n_1+n_2-4)\{(n_1-3)(n_2-2) + (n_2-3)\}]\sqrt{13} \\ &+ [\frac{1}{2}(n_1-2)(n_2-3)(n_2-4)+ \\ &\frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 + (n_1-3)(n_2-2)(n_2-3)]3\sqrt{2}.\end{aligned}$$

□

Theorem 4.2 *Let P_{n_1} and C_{n_2} with $n_1 \geq 3, n_2 \geq 4$ be path graph and cycle graph respectively, then*

$$\begin{aligned}\overline{RSO}(P_{n_1} \Box C_{n_2}) =& 2\sqrt{2}[n_2(n_2-3) + n_2^2] + 2n_2\sqrt{13}[n_2(n_1-2) - 1] \\ &+ 3\sqrt{2}[\frac{1}{2}(n_1n_2 - 2n_2 - 2)(n_1n_2 - 2n_2 - 3) + (n_2-3)].\end{aligned}$$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(C_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and C_{n_2} respectively. Based on degree of each vertex of the graph $P_{n_1} \Box C_{n_2}$, we obtain the fallowing number of non adjacent edges, as shown in the following table.

$(d(u), d(v))$	Number of non-adjacent edges
(3,3)	$n_2(n_2-3) + n_2^2$
(3,4)	$2n_2[n_2(n_1-2) - 1]$
(4,4)	$\frac{1}{2}(n_1n_2 - 2n_2 - 2)(n_1n_2 - 2n_2 - 3) + (n_2-3)$

By the definition, we have

$$\overline{RSO}(P_{n_1} \Box C_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l) \notin E(P_{n_1} \Box C_{n_2})} \sqrt{[d_{P_{n_1} \Box C_{n_2}}(u_i, v_j) - 1]^2 + [d_{P_{n_1} \Box C_{n_2}}(u_k, v_l) - 1]^2}$$

$$\overline{RSO}(P_{n_1} \Box C_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l) \notin E(P_{n_1} \Box C_{n_2})} \sqrt{[(d_{P_{n_1}}(u_i) + d_{C_{n_2}}(v_j)) - 1]^2 + [(d_{P_{n_1}}(u_k) + d_{C_{n_2}}(v_l)) - 1]^2}$$

Using above table, on simplification, we get

$$\begin{aligned}\overline{RSO}(P_{n_1} \Box C_{n_2}) =& 2\sqrt{2}[n_2(n_2-3) + n_2^2] + 2n_2\sqrt{13}[n_2(n_1-2) - 1] \\ &+ 3\sqrt{2}[\frac{1}{2}(n_1n_2 - 2n_2 - 2)(n_1n_2 - 2n_2 - 3) + (n_2-3)].\end{aligned}$$

□

Theorem 4.3 *If $P_{n_1} \boxtimes P_{n_2}$ is the strong product of two paths P_{n_1} and P_{n_2} then*
(i) $\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) = 8\sqrt{2} + 8(n_2-3)\sqrt{20} + (n_2-3)(n_2-4)8\sqrt{2}$ *for* $n_1 = 2$ *and* $n_2 \geq 3$
(ii) $\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) = 8\sqrt{2} + 8(n_1-3)\sqrt{20} + (n_1-3)(n_1-4)8\sqrt{2}$ *for* $n_1 \geq 3$ *and* $n_2 = 2$
(iii)

$$\begin{aligned}\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) =& 12\sqrt{2} + 8(n_1+n_2-5)\sqrt{20} + [(n_1-3)(2n_1-3)\\ &+ (2n_2-5)(2n_1+n_2-7)]4\sqrt{2} + 4[n_1n_2 - 2(n_1+n_2)+3]\sqrt{53}\\ &+ [2(n_1-3)\{(n_1-4)+(n_2-2)^2\} + 2(n_2-3)\{(n_2-4)+(n_1-2)^2\}]\sqrt{65}\\ &+ [\frac{1}{2}(n_1-2)(n_2-3)(n_2-4) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2\\ &+ (n_1-3)(n_2-3)(n_2-4)]7\sqrt{2}\, for\, n_1, n_2 \geq 3.\end{aligned}$$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(P_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and P_{n_2} respectively. Based on the degree of each vertex of the graph $P_{n_1} \boxtimes P_{n_2}$, we obtain the fallowing number of non adjacent edges, as shown in the following table

$P_{n_1} \boxtimes P_{n_2}$	$(d(u), d(v))$	Number of non-adjacent edges
$n_1 = 2, n_2 \geq 3$	(3,3)	4
	(3,5)	$8(n_2-3)$
	(5,5)	$2(n_2-3)(n_2-4)$
$n_1 \geq 3, n_2 = 2$	(3,3)	4
	(3,5)	$8(n_1-3)$
	(5,5)	$2(n_1-3)(n_1-4)$
$n_1, n_2 \geq 3$	(3,3)	6
	(3,5)	$8(n_1+n_2-5)$
	(5,5)	$(n_1-3)(2n_1-3) + (2n_2-5)(2n_1+n_2-7)$
	(3,8)	$4[n_1n - 2(n_1+n_2)+3]$
	(5,8)	$2(n_1-3)[(n_1-4)+(n_2-2)^2] + 2(n_2-3)[(n_2-4)+(n_1-2)^2]$
	(8,8)	$\frac{1}{2}(n_1-2)(n_2-3)(n_2-4) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2$ $+(n_1-3)(n_2-3)(n_2-4)$

By the definition, we have

$$\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l) \notin E(P_{n_1} \boxtimes P_{n_2})} \sqrt{[d_{P_{n_1} \boxtimes P_{n_2}}(u_i,v_j) - 1]^2 + [d_{P_{n_1} \boxtimes P_{n_2}}(u_k,v_l) - 1]^2}$$

Using the above table, on simplification, we get
(*i*) $\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) = 8\sqrt{2} + 8(n_2-3)\sqrt{20} + (n_2-3)(n_2-4)8\sqrt{2}$
(*ii*) $\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) = 4\sqrt{2} + 8(n_1-3)\sqrt{20} + (n_1-3)(n_1-4)8\sqrt{2}$
(*iii*)

$$\begin{aligned}\overline{RSO}(P_{n_1} \boxtimes P_{n_2}) &= 8\sqrt{2} + 8(n_1+n_2-5)\sqrt{20} + [(n_1-3)(2n_1-3) + (2n_2-5)(2n_1+n_2-7)]4\sqrt{2} \\ &+ 4[n_1n_2 - 2(n_1+n_2) + 3]\sqrt{53} + 2(n_1-3)[(n_1-4) + (n_2-2)^2]\sqrt{65} + \\ &2(n_2-3)[(n_2-4) + (n_1-2)^2]\sqrt{65} \\ &+ [\frac{1}{2}(n_1-2)(n_2-3)(n_2-4) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 + (n_1-3)(n_2-3)(n_2-4)]2\sqrt{7}.\end{aligned}$$

□

Theorem 4.4 *Let P_{n_1} and C_{n_2} with $n_1, n_2 \geq 4$, be path graph and cycle graph respectively then* $\overline{RSO}(P_{n_1} \boxtimes C_{n_2}) = 4\sqrt{2}[n_2(2n_2-3)] + 2n_2\sqrt{65}[n_2(n_1-2)] + 7\sqrt{2}[\frac{1}{2}\{n_2^2(n_1^2 - 4n_1 + 4) + 3n_2(8-3n_1)\}]$.

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(C_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and C_{n_2} respectively. Based on the degrees of each vertex of the graph $P_{n_1} \boxtimes C_{n_2}$, we obtain the fallowing number of non adjacent edges, as shown in the following table.

$(d(u), d(v))$	Number of non-adjacent edges
(5,5)	$n_2(2n_2-3)$
(5,8)	$2n_2[n_2(n_1-2)-3]$
(8,8)	$\frac{1}{2}[n_2^2(n_1^2 - 4n_1 + 4) + 3n_2(8-3n_1)]$

By the definition, we have

$$\overline{RSO}(P_{n_1} \boxtimes C_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l) \notin E(P_{n_1} \boxtimes C_{n_2})} \sqrt{[d_{P_{n_1} \boxtimes C_{n_2}}(u_i,v_j) - 1]^2 + [d_{P_{n_1} \boxtimes C_{n_2}}(u_k,v_l) - 1]^2}$$

Using the above table, on simplification, we get

$$\overline{RSO}(P_{n_1} \boxtimes C_{n_2}) = 4\sqrt{2}[n_2(2n_2-3)] + 2n_2\sqrt{65}[n_2(n_1-2)] + 7\sqrt{2}[\frac{1}{2}\{n_2^2(n_1^2 - 4n_1 + 4) + 3n_2(8-3n_1)\}].$$

□

Theorem 4.5 *If $P_{n_1} \otimes P_{n_2}$ is the direct product of two paths P_{n_1} and P_{n_2} then*
(*i*) $\overline{RSO}(P_{n_1} \otimes P_{n_2}) = 4(2n_2-5) + [(n_2-3)(2n_2-5)+1]\sqrt{2}$ *for $n_1 = 2$ and $n_2 > 2$*
(*ii*) $\overline{RSO}(P_{n_1} \otimes P_{n_2}) = 4(2n_1-5) + [(n_1-3)(2n_1-5)+1]\sqrt{2}$ *for $n_2 = 2$ and $n_1 > 2$*

(iii) For $n_1, n_2 \geq 3$

$$\begin{aligned}\overline{RSO}(P_{n_1} \otimes P_{n_2}) =& 8(n_1 + n - 4) + [(n_1+1)(n_1-3) + (n_1-2)(n_1+3n-11) \\ &+ (n_2-1)(n_2-3) + (n_2-2)(n_1+n_2-5)]\sqrt{2} + 12[(n_1-3)(n_2-2) + (n_2-3)] \\ &+ [(n_1-3)(n_2-2)(2n_2-4) + (n_2-3)(n_1-2)(2n_1-4) + 2(n_1-4)^2 + 2(n_2-4)^2 \\ &+ 4(n_1+n_2-6)]\sqrt{10} + [\frac{1}{2}(n_1-2)(n_2-2)(n_2-3) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 \\ &+ (n_1-3)2(n_2-3)(n_2-4)^2]3\sqrt{2}.\end{aligned}$$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(P_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and P_{n_2} respectively. Based on the degrees of each vertex of the graph $P_{n_1} \otimes P_{n_2}$, we obtain the fallowing number of non adjacent edges, as shown in the following table

$P_{n_1} \otimes P_{n_2}$	$(d(u), d(v))$	Number of non-adjacent edges
$n_1 = 2, n_2 > 2$	(1,1)	6
	(1,2)	$4(2n_2 - 5)$
	(2,2)	$(n_2-3)(2n_2-5)+1$
$n_1 = 2, n_2 > 2$	(1,1)	6
	(1,2)	$4(2n_2 - 5)$
	(2,2)	$(n_2-3)(2n_2-5)+1$
$n_1, n_2 \geq 3$	(1,1)	6
	(1,2)	$8(n_1+n_2-4)$
	(2,2)	$(n_1+1)(n_1-3)+(n_1-2)(n_1+3n_2-11)+(n_2-1)(n_2-3)$ $+(n_2-2)(n_1+n_2-5)$
	(1,4)	$4(n_1-3)(n_2-2)(n_2-3)$
	(2,4)	$(n_1-3)(n_2-2)(2n_2-4)+(n_2-3)(n_1-2)(2(n_1-4)$ $+2((n_1-4)^2+2(n_2-4)^2+4(n_1+n_2-6)$
	(4,4)	$\frac{1}{2}(n_1-2)(n_2-2)(n_2-3)+\frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2$ $+(n_1-3)2(n_2-3)(n_2-4)^2$

By the definition, we have

$$\overline{RSO}(P_{n_1} \otimes P_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l)\notin E(P_{n_1}\otimes P_{n_2})} \sqrt{[d_{P_{n_1}\otimes P_{n_2}}(u_i,v_j)-1]^2 + [d_{P_{n_1}\otimes P_{n_2}}(u_k,v_l)-1]^2}$$

Using the above table, we get
(i) $\overline{RSO}(P_{n_1} \otimes P_{n_2}) = 4(2n_2-5) + [(n_2-3)(2n_2-5)+1]\sqrt{2}$
(ii) $\overline{RSO}(P_{n_1} \otimes P_{n_2}) = 4(2n_1-5) + [(n_1-3)(2n_1-5)+1]\sqrt{2}$

$$\begin{aligned}(iii)\overline{RSO}(P_{n_1} \otimes P_{n_2}) =& 8(n_1+n-4) + [(n_1+1)(n_1-3) + (n_1-2)(n_1+3n-11) \\ &+ (n_2-1)(n_2-3) + (n_2-2)(n_1+n_2-5)]\sqrt{2} + 12[(n_1-3)(n_2-2)+(n_2-3)] \\ &+ [(n_1-3)(n_2-2)(2n_2-4) + (n_2-3)(n_1-2)(2n_1-4) + 2(n_1-4)^2 + 2(n_2-4)^2 \\ &+ 4(n_1+n_2-6)]\sqrt{10} + [\frac{1}{2}(n_1-2)(n_2-2)(n_2-3) + \frac{1}{2}(n_1-3)(n_1-4)(n_2-2)^2 \\ &+ (n_1-3)2(n_2-3)(n_2-4)^2]3\sqrt{2}.\end{aligned}$$

□

Theorem 4.6 *Let P_{n_1} and C_{n_2} with $n_1, n_2 \geq 3$ be path graph and cycle graph respectively, then*

$$\begin{aligned}\overline{RSO}(P_{n_1} \otimes C_{n_2}) = & n_2(2n_2-1)\sqrt{2} + n_2[n_1n_2 - 2(n_2+1)]\sqrt{10}+ \\ & \frac{1}{2}[(n_1n_2-3n_2)(n_1n_2-n_2-5) + n_2(n_2-1)]3\sqrt{2}.\end{aligned}$$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(C_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and C_{n_2} respectively. Based on the degree of each vertex of the graph $P_{n_1} \otimes C_{n_2}$, we obtain the fallowing number of non adjacent edges, as shown in the following table.

$(d(u), d(v))$	Number of non-adjacenct edges
(2,2)	$n_2(2n_2-1)$
(2,4)	$2n_2[n_1n_2 - 2(n_2+1)]$
(4,4)	$\frac{1}{2}[(n_1n_2-3n_2)(n_1n_2-n_2-5) + n_2(n_2-1)]$

By the definition

$$\overline{RSO}(P_{n_1} \otimes C_{n_2}) = \sum_{(u_i,v_j)(u_k,v_l)\notin E(P_{n_1}\otimes C_{n_2})} \sqrt{[d_{P_{n_1}\otimes C_{n_2}}(u_i,v_j)-1]^2 + [d_{P_{n_1}\otimes C_{n_2}}(u_k,v_l)-1]^2}$$

using the above table, on simplification, we get
$\overline{RSO}(P_{n_1} \otimes C_{n_2}) = n_2(2n_2-1)\sqrt{2} + n_2[n_1n_2 - 2(n_2+1)]\sqrt{10}$
$+\frac{1}{2}[(n_1n_2-3n_2)(n_1n_2-n_2-5) + n_2(n_2-1)]3\sqrt{2}.$

□

Theorem 4.7 *If $P_{n_1}[P_{n_2}]$ is the Lexicographic product of two paths P_{n_1} and P_{n_2} then*
(i) $\overline{RSO}(P_{n_1}[P_{n_2}]) = 4(n_2-3)\sqrt{n_2{}^2+(n_2{}^2+1)^2} + 2n_2\sqrt{2} + (n_2-3)(n_2-4)](n_2+1)\sqrt{2}$
for $n_1 = 2$ *and* $n_2 \geq 3$
(ii)

$$\begin{aligned}\overline{RSO}(P_{n_1}[P_{n_2}]) =& 4(2n_2-5) + 6(2n_2)\sqrt{2} + [(n_1-3)(2n_2-5)+1](n_2+1)\sqrt{2}\\ &+ [2(n_1-2)(n_2-3) + (n_1-3)(n_1-4)(n_2-2)]\sqrt{(2n_2)^2+(2n_2+1)^2}\\ &+ [(n_1-2)+(n_1-3)(n_1-4)]2n_2\sqrt{2}\\ &+ \frac{1}{2}[(n_1-2)(n_2-3)(n_2-4) + (n_2-2)^2(n_1-3)(n_1-4)](2n_2+1)\sqrt{2}\\ &for\, n_1, n_2 \geq 3.\end{aligned}$$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(P_{n_2}) = \{v_1, v_2, \cdots, v_{n_2}\}$ be the vertex sets of P_{n_1} and P_{n_2} respectively. Based on the degrees of each vertex of the graph $P_{n_1}[P_{n_2}]$, we obtain the fallowing number of non adjacent edges, as shown in the following table.

$P_{n_1}[P_{n_2}]$	$(d(u), d(v))$	Number of non-adjacent edges
$n_1 = 2, n_2 \geq 3$	(n_2+1, n_2+2)	$4(n_2-3)$
	(n_2+1, n_2+1)	2
	(n_2+2, n_2+2)	$(n_2-3)(n_2-4)$
$n_1, n_2 \geq 3$	(n_2+1, n_2+1)	$4(2n_2-5)$
	(n_2+1, n_2+1)	6
	(n_2+2, n_2+2)	$(n_1-3)(2n_2-5)+1$
	$(2n_2+1, 2n_2+2)$	$2(n_1-2)(n_2-3) + (n_1-3)(n_1-4)(n_2-2)$
	$(2n_2+1, 2n_2+1)$	$(n_1-2)+(n_1-3)(n_1-4)$
	$(2n_2+2, 2n_2+2)$	$\frac{1}{2}[(n_1-2)(n_2-3)(n_2-4) + (n_2-2)^2(n_1-3)(n_1-4)]$

By the definition, we have

$$\overline{RSO}(P_{n_1}[P_{n_2}]) = \sum_{(u_i,v_j)(u_k,v_l)\notin E(P_{n_1}[P_{n_2}])} \sqrt{[d_{P_{n_1}[P_{n_2}]}(u_i,v_j)-1]^2 + [d_{P_{n_1}[P_{n_2}]}(u_k,v_l)-1]^2}$$

Using the above table, on simplification, we get
(i) $\overline{RSO}(P_{n_1}[P_{n_2}]) = 4(n_2-3)\sqrt{n_2{}^2+(n_2+1)^2} + 2n_2\sqrt{2} + [(n_2-3)(n_2-4)](n_2+1)\sqrt{2}$

$$\begin{aligned}(ii)\overline{RSO}(P_{n_1}[P_{n_2}]) =& 4(2n_2-5) + 6(2n_2)\sqrt{2} + [(n_1-3)(2n_2-5)+1](n_2+1)\sqrt{2}\\ &+ [2(n_1-2)(n_2-3) + (n_1-3)(n_1-4)(n_2-2)]\sqrt{2n_2^2+(2n_2+1)^2}\\ &+ [(n_1-2)+(n_1-3)(n_1-4)]2n_2\sqrt{2}\\ &+ \frac{1}{2}[(n_1-2)(n_2-3)(n_2-4) + (n_2-2)^2(n_1-3)(n_1-4)](2n_2+1)\sqrt{2}.\end{aligned}$$

□

Theorem 4.8 *Let P_{n_1} and C_{n_2} with $n_1, n_2 \geq 3$ be a path graph and cycle graph respectively then* $\overline{RSO}(P_{n_1}[C_{n_2}]) = n_2(n_2-1)\sqrt{2}(2n_2-3) + 2(n_1-3){n_2}^2\sqrt{(n_2+1)^2+(2n_2+1)^2}$ $+\frac{n_2}{2}[(n_1-2)(n_2-3)+n_2(n_1-3)(n_1-4)](2n_2+1)\sqrt{2}.$

Proof: Let $V(P_{n_1}) = \{u_1, u_2, \cdots, u_{n_1}\}$ and $V(C_{n_2}) = \{v_1, v_2, \cdots, v_{n_1}\}$ be the vertex sets of P_{n_1} and C_{n_2} respectively. Based on the degrees of each vertex of the graph $P_{n_1}[C_{n_2}]$, we obtain the fallowing number of non adjacent edges, as shown in the following table.

$(d(u), d(v))$	Number of non-adjacent edges
(n_2+2, n_2+2)	$n_2(2n_2-3)$
$(n_2+2, 2n_2+2)$	$2(n_1-3){n_2}^2$
$(2n_2+2, 2n_2+2)$	$\frac{n_2}{2}[(n_1-2)(n_2-3)+n_2(n_1-3)(n_1-4)]$

By the definition

$$\overline{RSO}(P_{n_1}[C_{n_2}]) = \sum_{(u_i,v_j)(u_k,v_l)\notin E(P_{n_1}[C_{n_2}])} \sqrt{[d_{(P_{n_1}[C_{n_2}])}(u_i,v_j)-1]^2+[d_{(P_{n_1}[C_{n_2}])}(u_k,v_l)-1]^2}$$

using the above table, on simplification, we get

$$\begin{aligned}\overline{RSO}(P_{n_1}[C_{n_2}]) &= n_2(2n_2-3)\sqrt{2} + 2(n_1-3){n_2}^2\sqrt{(n_2+1)^2+(2n_2+1)^2}\\ &+\frac{n_2}{2}[(n_1-2)(n_2-3)+n_2(n_1-3)(n_1-4)](2n_2+1)\sqrt{2}.\end{aligned}$$

□

5. Bounds on Reduced Sombor Coindex of Graph Operations

Theorem 5.1 *Let G_1 and G_2 be any two graphs on n_1, n_2 vertices and m_1 and m_2 edges respectively. Then*
$\overline{m}\sqrt{2}[(\delta_1+\delta_2)-1] \leq \overline{RSO}(G_1\Box G_2) \leq \overline{m}\sqrt{2}[(\Delta_1+\Delta_2)-1].$
Equality holds if the given graphs G_1 and G_2 are regular.

Proof: Let $V(G_1) = \{u_i | i = 1, 2, \cdots, n_1\}$ and $V(G_2) = \{v_j | j = 1, 2, \cdots, n_2\}$ be the vertex sets of G_1 and G_2 respectively. Let δ_i be the minimum degree and Δ_i be the maximum degree of the vertex of G_i, where $i = 1, 2$.
In $G_1\Box G_2, |V(G_1\Box G_2)| = n_1n_2$ and $|E(G_1\Box G_2)| = n_1m_2 + m_1n_2$ and the number of non-adjacent edges in $G_1\Box G_2$ is $\overline{m} = \binom{n_1n_2}{2} - (n_1m_2+m_1n_2)$.
By the definition of $\overline{RSO}(G)$, we have

$$\begin{aligned}
\overline{RSO}(G) &= \sum_{uv\notin E(G)} \sqrt{(d(u)-1)^2+(d(v)-1)^2} \\
\overline{RSO}(G_1\Box G_2) &= \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\Box G_2)} \sqrt{[d_{G_1\Box G_2}(u_i,v_j)-1]^2+[d_{G_1\Box G_2}(u_k,v_l)-1]^2} \\
&= \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\Box G_2)} \sqrt{[(d_{G_1}(u_i)+d_{G_2}(v_j))-1]^2+[(d_{G_1}(u_k)+d_{G_2}(v_l))-1]^2} \\
&\le \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\Box G_2)} \sqrt{[(\Delta_1+\Delta_2)-1]2+[(\Delta_1+\Delta_2)-1]2} \\
&\le \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\Box G_2)} \sqrt{2}[(\Delta_1+\Delta_2)-1] \\
&\le \overline{m}\sqrt{2}[(\Delta_1+\Delta_2)-1].
\end{aligned}$$

Equality holds if the given graphs G_1 and G_2 are regular.
Similarly, we follow the lower bound. Thus,
$\overline{m}\sqrt{2}[(\delta_1+\delta_2)-1] \le \overline{RSO}(G_1\Box G_2) \le \overline{m}\sqrt{2}[(\Delta_1+\Delta_2)-1]$.

□

Theorem 5.2 *Let G_1 and G_2 be any two graphs with $|V(G_1)| = n_1, |E(G_1)| = m_1$ and $|V(G_2)| = n_2, |E(G_2)| = m_2$ respectively. Then*
$\overline{m}\sqrt{2}[(n_2\delta_1+\delta_2)-1] \le \overline{RSO}(G_1[G_2]) \le \overline{m}\sqrt{2}[(n_2\Delta_1+\Delta_2)-1]$.
Equality holds if G_1 and G_2 are regular.

Proof: Let $V(G_1) = \{u_i | i = 1, 2, \ldots, n_1\}$ and $V(G_2) = \{v_j | j = 1, 2, \ldots, n_2\}$ be the vertex sets of G_1 and G_2 respectively. Let δ_i and Δ_i be the minimum degree and maximum degree of the vertex of G_i, where $i = 1, 2$.
In $G_1[G_2], |V(G_1[G_2])| = n_1n_2$ and $|E(G_1[G_2])| = n_1m_2 + m_1n_2^2$ and the number of non-adjacent edges in $G_1[G_2]$ is $\overline{m} = \binom{n_1n_2}{2} - \left(n_1m_2 + m_1n_2^2\right)$.
By the definition of $\overline{RSO}(G)$, we have

$$\begin{aligned}
\overline{RSO}(G) &= \sum_{uv\notin E(G)} \sqrt{(d(u)-1)^2+(d(v)-1)^2} \\
\overline{RSO}(G_1[G_2]) &= \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1[G_2])} \sqrt{[d_{G_1[G_2]}(u_i,v_j)-1]^2+[d_{G_1[G_2]}(u_k,v_l)-1]^2} \\
&\le \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1[G_2])} \sqrt{[(n_2\Delta_1+\Delta_2)-1]2+[(n_2\Delta_1+\Delta_2)-1]2} \\
&\le \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1[G_2])} \sqrt{2}[(n_2\Delta_1+\Delta_2)-1] \\
&\le \overline{m}\sqrt{2}[(n_2\Delta_1+\Delta_2)-1].
\end{aligned}$$

Equality holds if the given graphs G_1 and G_2 are regular.
Similarly, we follow the lower bound. Thus,
$\overline{m}\sqrt{2}[(n_2\delta_1+\delta_2)-1] \le \overline{RSO}(G_1[G_2]) \le \overline{m}\sqrt{2}[(n_2\Delta_1+\Delta_2)-1]$.

□

Theorem 5.3 *Let G_1 and G_2 be any two graphs with $|V(G_1)| = n_1, |E(G_1)| = m_1$ and $|V(G_2)| = n_2, |E(G_2)| = m_2$ respectively.*
Then $\overline{m}\sqrt{2}(\delta_1\delta_2 - 1) \leq \overline{RSO}(G_1 \otimes G_2) \leq \overline{m}\sqrt{2}(\Delta_1\Delta_2 - 1)$.
Equality holds if G_1 and G_2 are regular.

Proof: Let $V(G_1) = \{u_1, u_2, \ldots, u_{n1}\}$ and $V(G_2) = \{v_1, v_2, \ldots, v_{n2}\}$ be the disjoint vertex sets of G_1 and G_2 respectively. Let δ_i and Δ_i be the minimum degree and maximum degree of the vertex of G_i where $i = 1, 2$.
In $G_1 \otimes G_2, |V(G_1 \otimes G_2)| = n_1n_2$ and $|E(G_1 \otimes G_2)| = 2m_1m_2$ and the number of non-adjacent edges in $G_1 \otimes G_2$ is $\overline{m} = \begin{pmatrix} n_1n_2 \\ 2 \end{pmatrix} - 2m_1m_2$. By the definition of $\overline{RSO}(G)$, we have

$$\overline{RSO}(G_1 \otimes G_2) = \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\otimes G_2)} \sqrt{[d_{G_1\otimes G_2}(u_i, v_j) - 1]^2 + [d_{G_1\otimes G_2}(u_k, v_l) - 1]^2}$$

$$\begin{aligned}\overline{RSO}(G_1 \otimes G_2) &= \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\otimes G_2)} \sqrt{[(d_{G_1}(u_i)d_{G_2}(v_j)) - 1]^2 + [(d_{G_1}(u_k)d_{G_2}(v_l)) - 1]^2} \\ &\leq \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\otimes G_2)} \sqrt{(\Delta_1\Delta_2 - 1)^2 + (\Delta_1\Delta_2 - 1)^2} \\ &\leq \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\otimes G_2)} (\Delta_1\Delta_2 - 1)\sqrt{2} \\ &\leq \overline{m}\sqrt{2}(\Delta_1\Delta_2 - 1).\end{aligned}$$

Equality holds if the given graphs G_1 and G_2 are regular.
Similarly, we follow the lower bound.
Thus, $\overline{m}\sqrt{2}(\delta_1\delta_2 - 1) \leq \overline{RSO}(G_1 \otimes G_2) \leq \overline{m}\sqrt{2}(\Delta_1\Delta_2 - 1)$.

□

Theorem 5.4 *Let G_1 and G_2 be any two graphs on n_1 and n_2 vertices and m_1 and m_2 edges respectively. Then*
$\overline{m}\sqrt{2}[(\delta_1 + \delta_2 + \delta_1\delta_2) - 1] \leq \overline{RSO}(G_1 \boxtimes G_2) \leq \overline{m}\sqrt{2}[(\Delta_1 + \Delta_2 + \Delta_1\Delta_2) - 1]$.
Equality holds if G_1 and G_2 are regular.

Proof: Let $V(G_1) = \{u_1, u_2, \ldots, u_{n1}\}$ and $V(G_2) = \{v_1, v_2, \ldots, v_{n2}\}$ be the disjoint vertex sets of G_1 and G_2 respectively. Let δ_i and Δ_i be the minimum and maximun degree of the vertex of G_i where $i = 1, 2$.
In $G_1 \boxtimes G_2, |V(G_1 \boxtimes G_2)| = n_1n_2$ and $|E(G_1 \boxtimes G_2)| = n_1m_2 + m_1n_2 + 2m_1m_2$ and the number of non-adjacent edges in $G_1 \boxtimes G_2$ is $\overline{m} = \begin{pmatrix} n_1n_2 \\ 2 \end{pmatrix} - (n_1m_2 + m_1n_2 + 2m_1m_2)$.
By the definition of $\overline{RSO}(G)$, we have

$$\overline{RSO}(G) = \sum_{uv\notin E(G)} \sqrt{(d(u) - 1)^2 + (d(v) - 1)^2}$$

$$\begin{aligned}\overline{RSO}(G_1 \boxtimes G_2) &= \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\boxtimes G_2)} \sqrt{[d_{G_1\boxtimes G_2}(u_i, v_j) - 1]^2 + [d_{G_1\boxtimes G_2}(u_k, v_l) - 1]^2} \\ &\leq \sum_{(u_i,v_j)(u_k,v_l)\notin E(G_1\boxtimes G_2)} \sqrt{2}[(\Delta_1 + \Delta_2 + \Delta_1\Delta_2) - 1] \\ &\leq \overline{m}\sqrt{2}[(\Delta_1 + \Delta_2 + \Delta_1\Delta_2) - 1]\end{aligned}$$

Equality holds if the given graphs G_1 and G_2 are regular.
Similarly, we follow the lower bound. Thus,

$$\overline{m}\sqrt{2}[(\delta_1+\delta_2+\delta_1\delta_2)-1] \le \overline{RSO}(G_1 \boxtimes G_2) \le \overline{m}\sqrt{2}[(\Delta_1+\Delta_2+\Delta_1\Delta_2)-1].$$

□

6. Correlation Analysis with Some Selected Hetero Molecules

This section explores the chemical applicability of $\overline{RSO}(G)$ index through a correlation analysis, considering total π-electron energy of selected hetero molecules [2,11] as the dependent variable (Y) and the $\overline{RSO}(G)$ of the selected hetero molecules as the independent variable (X). The experimental values of the total π-electron energy and $\overline{RSO}(G)$ value for each selected hetero molecule is provided in Table 1 and corresponding correlation graph is shown in Figure1 .

Code of hetero molecules	$\overline{RSO}(G)$	**Total π-electron energy**
$H1$	0.5	2.23
$H2$	2.2071	5.66
$H3$	2.2071	5.76
$H5$	2.2071	6.82
$H6$	3.5355	5.23
$H7$	8.4853	6.69
$H8$	8.4853	9.06
$H9$	8.4853	9.1
$H10$	8.4853	9.07
$H11$	8.4853	9.65
$H12$	16.045	8.19
$H13$	25.04	12.21
$H14$	24.754	12.22
$H15$	24.754	12.21
$H16$	24.207	11
$H17$	41.751	14.23
$H18$	41.751	14.23
$H19$	56.79	16.15
$H20$	56.45	16.12
$H21$	31.152	13.46
$H22$	31.152	13.59
$H23$	98.306	20.1
$H24$	98.306	21.02
$H25$	97.618	20.56
$H26$	97.618	21.62
$H27$	139.55	24.23
$H28$	81.359	19.39

Table 1: $\overline{RSO}(G)$ value of selected hetero molecules and corresponding π-electron energy

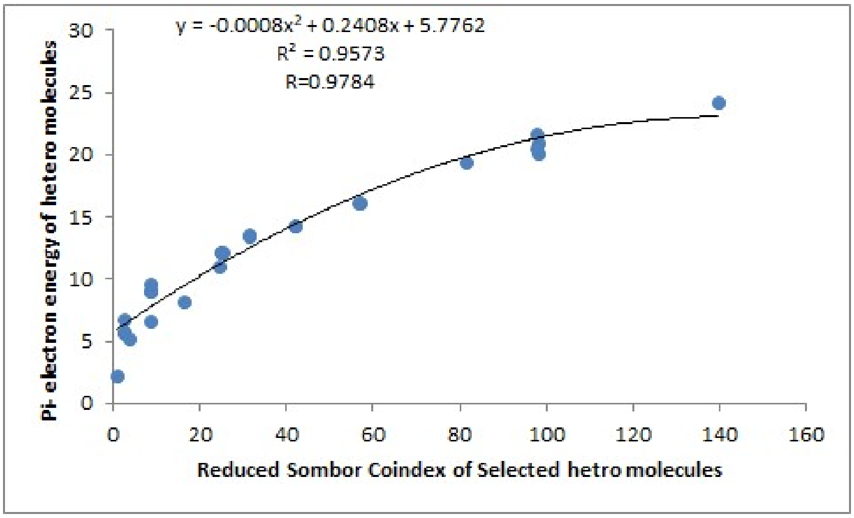

Figure 1: Correlation graph of selected hetero molecules

7. Correlation Analysis with Some Selected PAHs

This section explores the chemical applicability of $\overline{RSO}(G)$ index through correlation analysis, considering total π-electron energy of selected PAHs [2] as the dependent variable (Y) and the $\overline{RSO}(G)$ value of the selected PAHs as the independent variable (X). The Table 2 represents the experimental value of the total π-electron energy and $\overline{RSO}(G)$ value for each selected PAHs, Figure 2 shows the corresponding correlation graph.

PAHs	$\overline{RSO}(G)$	**Total π-electron energy**
Benzene	8.4853	8
Naphthalene	41.751	13.68
Phenanthrene	93.431	19.44
Anthracene	97.274	19.31
Chrysene	170.5	25.19
Benzanthracene	175.76	25.1
Benzo[a]pyrene	216.8	28.22
Perylene	216.8	28.24
Anthanthrene	268.76	31.25
Dibenzo(a, c)anthracene	276.52	30.94
Dibenzo(a, h)anthracene	276.53	30.88
Dibenzo(a, j)anthracene	270.2	30.94
Picene	327.45	33.95
Pyrene	128.42	22.5
Coronene	326.74	34.57
Fluoranthene	129.13	22.5
Pentacene	276.88	30.54

Table 2: $\overline{RSO}(G)$ value of selected PAHs and corresponding π-electron energy

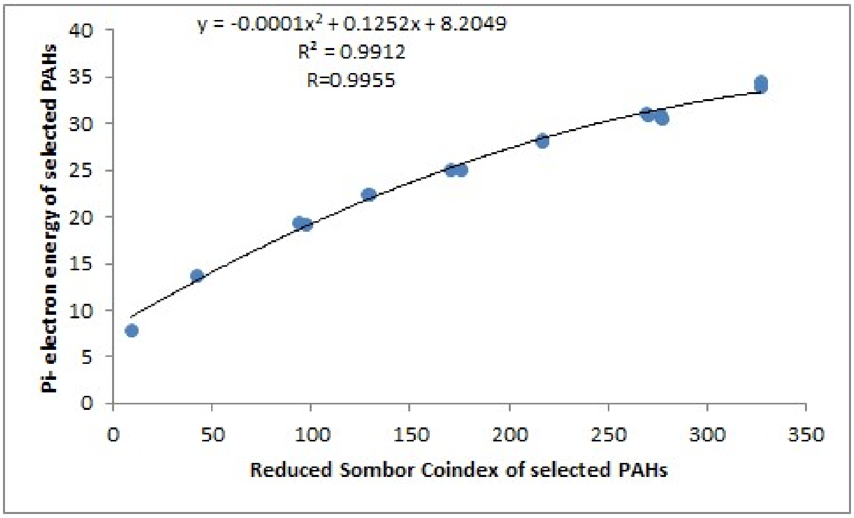

Figure 2: Correlation graph of selected PAHs

8. Conclusion

In this paper , we introduced new degree based coindex called reduced Sombor coindex for certain graphs like cycle graph, complete bipartite graph, wheel graph and path graphs. Further we extend this work to find reduced Sombor coindex of graph operations like cartesian product, strong product. direct product and lexicographic product of two graphs. As a part of extention of this work we compute some stong bounds of the reduced Sombor coindex. Further we discussed chemical applicability of reduce sombor coindex here we compared reduced sombar coindex values of certain hetero molecules with their total π-electron energy and it is found to be very good correlation of 0.9784. Also, we correlated reduce sombar coindex values of some selected PAHs with their total π-electron energy and the correlation co-efficient is 0.9955. That describes the high chemical applicability of this index.

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