International Journal of
Mathematics And its Applications
ISSN: 2347-1557

Int. J. Math. And Appl., **13(2)**(2025), 211–221
Available Online: http://ijmaa.in

More on KG Sombor Index of Graphs

Mitesh J. Patel[1,*], Kajal S. Baldaniya[2], Ashika Panicker[2]

[1] *Department of Mathematics, Tolani College of Arts and Science, Adipur, Gujarat, India*
[2] *Research Scholar, KSKV Kachchh University, Bhuj, Gujarat, India*

Abstract

Let $G = (V(G), E(G))$ be a graph of order n and size m. The KG Sombor index of graph G is defined as $KG(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2}$, where $\sum_{ue}$ indicates summation over vertices $u \in V(G)$ and the edges $e \in V(G)$ that are incident to u. In this paper, we found some useful correlation between KG Sombor index and dielectric constant as well as density of various organic hydrocarbons. We also derive some new bounds of KG Sombor index of graph with respect to different topological indices using mathematical inequities. Moreover we obtain KG Sombor index of corona product of two graphs.

Keywords: KG Sombor Index; Correlation; Dielectric constant; Corona product of two graphs.
2020 Mathematics Subject Classification: 05C50, 05C92.

1. Introduction

Let $G = (V(G), E(G))$ be a undirected, simple and connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of vertex $v \in V(G)$ is denoted by d_v is the number of edges incident with v. We denote $e = uv$ is the edge connecting the vertices u and v. The degree of an edge e is the number of edges that are incident to e is denoted by d_e, then $d_e = d_u + d_v - 2$. In this paper we consider graphs without loops and multiple edges. We follow Bondy and Murty [1] for standard terminology and notation in graph theory. We first recall the relevant vertex–degree–based graph invariants that we have used in this paper. In [2] and [3], the first and second Zagreb indices of graph $G = (V(G), E(G))$ are define as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) \quad and$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v).$$

*Corresponding author (miteshmaths1984@gmail.com)

In [4], the forgotten index of graph G is

$$F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2).$$

Considering the algebraic form of Zagreb indices, V. R. Kulli [5] have presented the first and second K Banhatti indices as

$$B_1(G) = \sum_{ue} (d_u + d_e) \quad and$$
$$B_2(G) = \sum_{ue} d_u d_e,$$

where $u \in V(G)$ and $e \in E(G)$are incident in G. Interestingly, in [6,7] the sum connectivity Banhatti index of graph G is defined as

$$ISB(G) = \sum_{ue} \sqrt{d_u + d_e}$$

and the product connectivity Banhatti index of graph G is defined as

$$IPB(G) = \sum_{ue} \sqrt{d_u d_e},$$

where $u \in V(G)$ and $e \in E(G)$ are incident in G. KG Sombor index was inspired from a very innovative degree of vertex-based topological index popularly known as Sombor index defined in [8] as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

Mathematical properties and interesting results on Sombor index are available in [9–12]. V. R. Kulli, et al. [13] define the KG Sombor index of graph G as

$$KG(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2},$$

where the above summation is over vertices $u \in V(G)$ and the edges $e \in E(G)$ that are incident to vertex u. They found KG-Sombor index of regular graph, complete bipartite graph and also derive some interesting bounds. I. Gutman, I. Redžepovi ́c and V. R. Kulli [14] derive some interesting results on KG-Sombor index of Kragujevac trees. If the sum is depends on edges $e = uv \in E(G)$ then

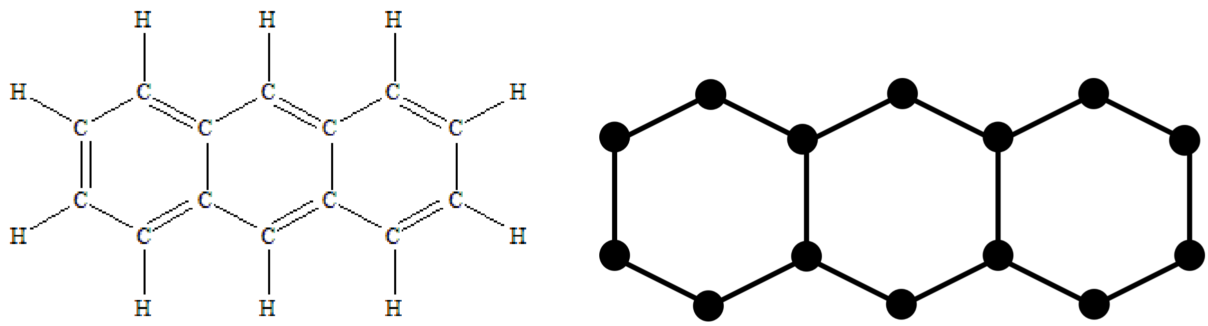
$$KG(G) = \sum_{e=uv \in E(G)} \left(\sqrt{d_u^2 + d_e^2} + \sqrt{d_v^2 + d_e^2} \right).$$

Definition 1.1 ([15]). *The dielectric constant of a substance can be defined as* $K = \frac{\epsilon}{\epsilon_0}$, *where* ϵ *is the permittivity of the substance and* ϵ_0 *is the permittivity of the free space.*

Definition 1.2 ([15]). *Density of a hydrocarbon is discussed as the ratio of mass and volume of a hydrocarbon.*

2. Relation Between KG Sombor Index and Coefficients of Hydrocarbons

We have evaluated KG Sombor indices of various aromatic hydocarbons like benzene, anthracene, phenanthrene, chrysene, coronene, etc and non aromatic hydrocarbons hexane, butadiene and paraxylene using the chemical structures and their respective graphs. Here, the carbon element is consider as a vertex and bonds between carbons is considered as an edge. Below Figure 1 is the chemical structure and related graph of hydrocarbon Anthracene.



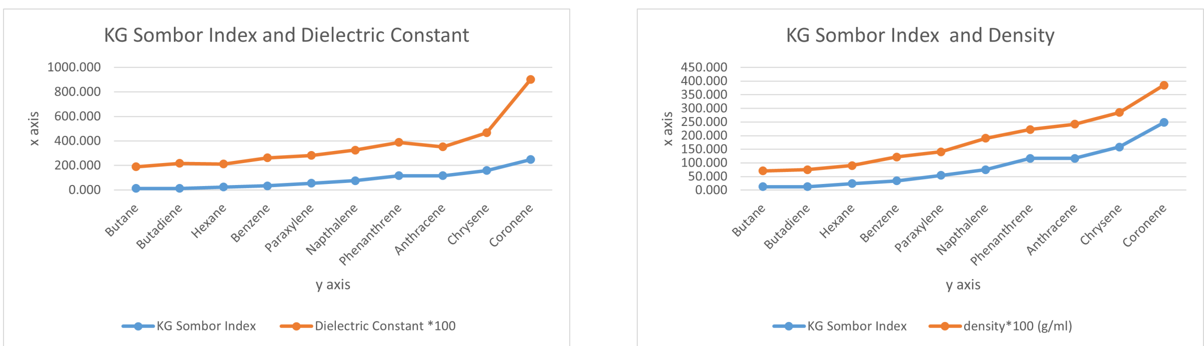
(a) The chemical structure of Anthracene (b) The graph of Anthracene

Figure 1

From [16], the dielectric constant of Anthracene is 2.59 and density is $1.25 g/cm^3$. Let G be a graph derived from Anthracene molecule. Then

$$\begin{aligned} KG(G) &= \sum_{e=uv\in E(G)} \left(\sqrt{d_u^2+d_e^2}+\sqrt{d_v^2+d_e^2}\right) \\ &= 12\sqrt{2^2+2^2}+8\sqrt{2^2+3^2}+8\sqrt{3^2+3^2}+4\sqrt{3^2+4^2}=116.72. \end{aligned}$$

Using which, a remarkable correlation of the KG Sombor index with the dielectric constant and density of the hydrocarbons compound has been observed. The correlation coefficient of KG Sombor index with the dielectric constant is 0.891862389, and the correlation coefficient of KG Sombor index with the density is 0.895463563.



(a) KG Sombor Index and Dielectric Constant (b) KG Sombor Index and Density

Figure 2

3. Bounds of KG Sombor Index

Lemma 3.1 ([17]). *Let a and b be any two real numbers. Then*

$$\frac{|a|+|b|}{\sqrt{2}} \leq \sqrt{a^2+b^2} \leq |a|+|b|.$$

Theorem 3.2. *Let G be a graph of order n and size m. Then*

$$\frac{1}{\sqrt{2}}(3M_1(G)-4m) \leq KG(G) \leq 3M_1(G)-4m.$$

Proof. By Lemma 3.1, for $a = d_u \geq 0$ and $b = d_e \geq 0$, we have

$$\frac{d_u+d_e}{\sqrt{2}} \leq \sqrt{d_u^2+d_e^2} \leq d_u+d_e$$

and for $a = d_v \geq 0$ and $b = d_e \geq 0$, we have

$$\frac{d_v+d_e}{\sqrt{2}} \leq \sqrt{d_v^2+d_e^2} \leq d_u+d_e.$$

Adding above both equations,

$$\begin{aligned}
\frac{d_u+d_e}{\sqrt{2}}+\frac{d_v+d_e}{\sqrt{2}} &\leq \sqrt{d_u^2+d_e^2}+\sqrt{d_v^2+d_e^2} \leq d_u+d_e+d_v+d_e \\
\Rightarrow \sum_{e=uv\in E(G)} \frac{d_u+d_e+d_v+d_e}{\sqrt{2}} &\leq KG(G) \leq \sum_{e=uv\in E(G)} (d_u+d_v+2d_e) \\
\Rightarrow \sum_{e=uv\in E(G)} \frac{d_u+d_v+2(d_u+d_v-2)}{\sqrt{2}} &\leq KG(G) \leq \sum_{e=uv\in E(G)} (d_u+d_v+2(d_u+d_v-2)) \\
\Rightarrow \frac{1}{\sqrt{2}}\big(3\sum_{e=uv\in E(G)}(d_u+d_v)-\sum_{e=uv\in E(G)}4\big) &\leq KG(G) \leq 3\sum_{e=uv\in E(G)}(d_u+d_v)-\sum_{e=uv\in E(G)}4 \\
\Rightarrow \frac{1}{\sqrt{2}}(3M_1(G)-4m) &\leq KG(G) \leq 3M_1(G)-4m.
\end{aligned}$$

Hence the result. □

Theorem 3.3. *Let G be a graph of order n, size m and with no pendent vertex. Then*

$$KG(G) \leq 2\sqrt{2}[M_1(G)-2m].$$

Proof. As per definition of KG Sombor index of graph G, we have

$$\begin{aligned}
KG(G) &= \sum_{uv\in E(G)} \big(\sqrt{d_u^2+d_e^2}+\sqrt{d_v^2+d_e^2}\,\big) \\
&= \sum_{e=uv\in E(G)} \big(\sqrt{\frac{1}{2}[(d_u-d_e)^2+(d_u+d_e)^2]}+\sqrt{\frac{1}{2}[(d_v-d_e)^2+(d_v+d_e)^2]}\,\big)
\end{aligned}$$

$$
\begin{aligned}
&\leq \frac{1}{\sqrt{2}} \sum_{e=uv\in E(G)} \big(|d_u - d_e| + |d_u + d_e| + |d_v - d_e| + |d_v + d_e|\ \big)\ (\because \textit{Lemma } 3)\\
&= \frac{1}{\sqrt{2}} \sum_{e=uv\in E(G)} \big(|d_v - 2| + |2d_u + d_v - 2| + |d_u - 2| + |d_u + 2d_v - 2|\ \big)\\
&= \frac{1}{\sqrt{2}} \sum_{e=uv\in E(G)} (4d_u + 4d_v - 8)\ (\because\ d_u, d_v \geq 2)\\
&= 2\sqrt{2} \sum_{e=uv\in E(G)} (d_u + d_v - 2)\\
&= 2\sqrt{2}[M_1(G) - 2m].
\end{aligned}
$$

Hence the result. □

Lemma 3.4 ([17]). *Cauchy Schwartz inequality: For real vectors $a = (a_1, a_2, \ldots, a_n)$ and $b = (b_1, b_2, \ldots, b_n)$,*

$$
\sum_{i=1}^{n} a_i b_i \leq \Big(\sum_{i=1}^{n} a_i^2\Big)^{1/2} \Big(\sum_{i=1}^{n} b_i^2\Big)^{1/2}.
$$

Theorem 3.5. *Let G be a graph of order n and size m. Then*

$$
KG(G) \leq 2\sqrt{m(F(G) + 2M_2(G) - 3M_1(G) + 4m)}.
$$

Proof. By Cauchy Schwartz inequality, for $a_i = 1$ and $b_i = \sqrt{d_u^2 + d_e^2}$ we have

$$
\begin{aligned}
\Bigg(\sum_{e=uv\in E(G)} 1 \cdot \sqrt{d_u^2 + d_e^2}\Bigg)^2 &\leq \sum_{e=uv\in E(G)} 1^2 \sum_{e=uv\in E(G)} (d_u^2 + d_e^2)\\
&= m \sum_{e=uv\in E(G)} \Big(d_u^2 + (d_u + d_v - 2)^2\Big)\\
&= m \sum_{e=uv\in E(G)} \Big(d_u^2 + d_u^2 + d_v^2 + 4 + 2d_u d_v - 4d_u - 4d_v\Big)\\
&= m\Big[\sum_{e=uv\in E(G)} d_u^2 + \sum_{e=uv\in E(G)} (d_u^2 + d_v^2) + 2\sum_{e=uv\in E(G)} d_u d_v\\
&\qquad - 4\sum_{e=uv\in E(G)} (d_u + d_v + 1)\Big]\\
&= m\Big[M_1(G) + F(G) + 2M_2(G) - 4M_1(G) + 4m\Big]\\
\Rightarrow \sum_{e=uv\in E(G)} \sqrt{d_u^2 + d_e^2} &\leq \Big[m\Big(F(G) + 2M_2(G) - 3M_1(G) + 4m\Big)\Big]^{\frac{1}{2}}.
\end{aligned}
$$

Similarly,

$$
\sum_{e=uv\in E(G)} \sqrt{d_v^2 + d_e^2} \leq \Big[m\Big(F(G) + 2M_2(G) - 3M_1(G) + 4m\Big)\Big]^{\frac{1}{2}}.
$$

Therefore,

$$KG(G) = \sum_{e=uv\in E(G)} \sqrt{d_u^2 + d_e^2} + \sqrt{d_v^2 + d_e^2} \leq 2\sqrt{m\Big(F(G) + 2M_2(G) - 3M_1(G) + 4m\Big)}.$$

Hence the result. □

Theorem 3.6. *Let G be a graph of order n and size m. Then*

$$KG(G) + KG(\overline{G}) \leq n(n-1)\sqrt{5n^2 - 18n + 17},$$

equality satisfies if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

Proof. Let G be a graph of order n and the maximum degree of vertex in G is Δ. Then

$$\Delta \leq n - 1 \Rightarrow d_u \leq n - 1,$$

for every vertex u. The degree of an edge $e = uv$ is $d_e = d_u + d_v - 2 \Rightarrow d_e \leq 2(n-2)$. So for any edge $e = uv$, it is easy to verify that

$$\sqrt{d_u^2 + d_e^2} + \sqrt{d_v^2 + d_e^2} \leq 2\sqrt{(n-1)^2 + 4(n-2)^2}.$$

so,

$$\begin{aligned} KG(G) + KG(\overline{G}) &= \sum_{e=uv\in E(G)} \left(\sqrt{d_u^2 + d_e^2} + \sqrt{d_v^2 + d_e^2}\right) + \sum_{e=uv\in E(\overline{G})} \left(\sqrt{d_u^2 + d_e^2} + \sqrt{d_v^2 + d_e^2}\right) \\ &\leq \sum_{e=uv\in E(G)} 2\sqrt{(n-1)^2 + 4(n-2)^2} + \sum_{e=uv\in E(\overline{G})} 2\sqrt{(n-1)^2 + 4(n-2)^2}. \end{aligned}$$

Since, $|E(G)| + |E(\overline{G})| = \frac{n(n-1)}{2}$, we obtain

$$\begin{aligned} KG(G) + KG(\overline{G}) &\leq \frac{n(n-1)}{2} \times 2\sqrt{(n-1)^2 + 4(n-2)^2} \\ &= n(n-1)\sqrt{5n^2 - 18n + 17}. \end{aligned}$$

Additionally, the equality is satisfied if and only if $G \cong K_n$ or $G \cong \overline{K}_n$. In [13] the KG Sombor index of $r-$regular graph G of order n is $KG(G) = nr\sqrt{5r^2 - 8r + 4}$. To verify put $r = n - 1$ for complete graph K_n and $r = 0$ for graph $\overline{K}_n$. □

Lemma 3.7 ([17]). *Let p, q, r and s be any real numbers satisfying $p \geq q \geq r \geq s \geq 0$. Then*

$$\sqrt{p + r} + \sqrt{q + s} \geq \sqrt{p + q} + \sqrt{r + s}.$$

Theorem 3.8. *Let G be a graph of size m. Then $KG(G) \geq \sqrt{2}M_1 - 2\sqrt{2}m + SO(G)$.*

Proof. By Lemma 3.7, for, $p = q = d_e^2 \geq r = d_u \geq s = d_v^2$, we have

$$\begin{aligned}
\sqrt{d_e^2 + d_u^2} + \sqrt{d_e^2 + d_v^2} &\geq \sqrt{2d_e^2} + \sqrt{d_u^2 + d_v^2} \\
\Rightarrow \sum_{e=uv\in E(G)} \left(\sqrt{d_e^2 + d_u^2} + \sqrt{d_e^2 + d_v^2}\right) &\geq \sum_{e=uv\in E(G)} \sqrt{2}d_e + \sum_{e=uv\in E(G)} \sqrt{d_u^2 + d_v^2} \\
\Rightarrow KG(G) &\geq \sqrt{2} \sum_{e=uv\in E(G)} (\ d_u + d_v - 2) \ + SO(G) \\
\Rightarrow KG(G) &\geq \sqrt{2}M_1 - 2\sqrt{2}m + SO(G).
\end{aligned}$$

Hence the result. □

Theorem 3.9. *Let G be a graph. Then $KG(G) \geq \sqrt{2B_2(G)}$.*

Proof. For positive real numbers a and b, we have

$$\frac{a}{b} + \frac{b}{a} \geq 2.$$

Consider $a = d_u$ and $b = d_e$ then inequity becomes

$$\begin{aligned}
\frac{d_u}{d_e} + \frac{d_e}{d_u} &\geq 2 \\
\Rightarrow \sqrt{d_u^2 + d_e^2} &\geq \sqrt{2d_e d_u} \\
\Rightarrow \sum_{ue} \sqrt{d_u^2 + d_e^2} &\geq \sum_{ue} \sqrt{2d_e d_u} \\
\Rightarrow KG(G) &\geq \sqrt{2B_2(G)}.
\end{aligned}$$

This can be equivalently understood from [7] as $KG(G) \geq \sqrt{2}IPB(G)$. □

4. KG Sombor Index of Corona Product of graphs

Definition 4.1 ([18])**.** *The corona product $G \circ H$ of two graphs G and H is obtained by taking one copy of G and $|V(G)|$ copies of H and making the i^{th} vertex of G adjacent to each vertex of the i^{th} copy of H, where $1 \leq i \leq |V(G)|$. Here G is called the center graph and H is called the outer graph.*

Theorem 4.2. *Let G be a $r-$regular graph. Then KG Sombor index of corona product of G with complete graph K_1 is*

$$KG(G \circ K_1) = n\left[r\sqrt{5r^2 + 2r + 1} + \sqrt{2r^2 + 2r + 1} + \sqrt{r^2 + 1}\right].$$

Proof. Consider $r-$regular graph G with n vertices $u_1, u_2, \ldots, u_n$ and complete graph K_1. For corona product $G \circ K_1$ we attach n pendent vertices $v_1, v_2, \ldots v_n$ to corresponding vertices of G. Now in $G \circ K_1$,

$d(u_i) = r+1$ and $d(v_i) = 1$ for every $i = 1, 2, \ldots, n$. The KG Sombor index of $G \circ K_1$ is

$$\begin{aligned} KG(G \circ K_1) &= 2 \sum_{u_i u_j, i \neq j} \sqrt{(r+1)^2 + (2r)^2} + \sum_{u_i v_i} \sqrt{(r+1)^2 + (r)^2} + \sum_{u_i v_j} \sqrt{1 + r^2} \\ &= nr\sqrt{5r^2 + 2r + 1} + n\sqrt{2r^2 + 2r + 1} + n\sqrt{r^2 + 1} \\ &= n\left[r\sqrt{5r^2 + 2r + 1} + \sqrt{2r^2 + 2r + 1} + \sqrt{r^2 + 1}\right]. \end{aligned}$$

Hence the result. □

Corollary 4.3. *KG Sombor index of corona product of cycle C_n with K_1 is*

$$KG(C_n \circ K_1) = \left(10 + \sqrt{13} + \sqrt{5}\right) n.$$

Corollary 4.4. *KG Sombor index of corona product of complete graph K_n with K_1 is*

$$KG(K_n \circ K_1) = n\left[(n-1)\sqrt{5n^2 - 8n + 4} + \sqrt{2n^2 - 2n + 1} + \sqrt{n^2 - 2n + 2}\right].$$

Corollary 4.5. *KG Sombor index of corona product of generalized peterson graph $P(n,k)$ with K_1 is*

$$KG(P(n,k) \circ K_1) = n\left[5 + 2\sqrt{13} + \sqrt{10}\right].$$

Theorem 4.6. *KG Sombor index of path graph P_n with complete graph K_1 is*

$$KG(P_n \circ K_1) = \left(10 + \sqrt{13} + \sqrt{5}\right) n + 8\sqrt{2} - 30.$$

Proof. Let $u_1, u_2, \ldots u_n$ be n vertices of path P_n with $d(u_i) = 2$, where $i = 2, 3, \ldots, n-1$ and $d(u_1) = d(u_n) = 1$. The corona product $P_n \circ K_1$ is obtained by connecting n pendent vertices $v_1, v_2, \ldots v_n$ to corresponding vertices of path P_n. The KG Sombor index of $P_n \circ K_1$ is

$$\begin{aligned} KG(P_n \circ K_1) = &\sum_{u_i u_j, i,j \neq 1,n} \left(\sqrt{(d_{u_i}+1)^2 + (d_{u_i} + d_{u_j})^2} + \sqrt{(d_{u_j}+1)^2 + (d_{u_i} + d_{u_j})^2}\right) \\ &+ \sum_{u_i v_i, i \neq 1,n} \left(\sqrt{(d_{u_i}+1)^2 + (d_{u_i} + 1 + d_{v_i} - 2)^2} + \sqrt{(d_{v_i})^2 + (d_{u_i} + 1 + d_{v_i} - 2)^2}\right) \\ &+ \sum_{u_i u_j, i=1,n-1, j=i+1} \left(\sqrt{(d_{u_i}+1)^2 + (d_{u_i} + d_{u_j})^2} + \sqrt{(d_{u_j}+1)^2 + (d_{u_i} + d_{u_j})^2}\right) \\ &+ \sum_{u_i v_i, i=1,n} \left(\sqrt{(d_{u_i}+1)^2 + (d_{u_i} + 1 + d_{v_i} - 2)^2} + \sqrt{(d_{v_i})^2 + (d_{u_i} + 1 + d_{v_i} - 2)^2}\right) \\ = &\sum_{u_i u_j, i,j \neq 1,n} \left(2\sqrt{9+16}\right) + \sum_{u_i v_i, i \neq 1,n} \left(\sqrt{9+4} + \sqrt{1+4}\right) \\ &+ \sum_{u_i u_j, i=1,n-1, j=i+1} \left(\sqrt{4+9} + \sqrt{9+9}\right) + \sum_{u_i v_i, i=1,n} \left(\sqrt{4+1} + \sqrt{1+1}\right). \end{aligned}$$

$$= 10(n-3) + \left(\sqrt{13}+\sqrt{5}\right)(n-2) + \left(\sqrt{13}+3\sqrt{2}\right)(2) + \left(\sqrt{5}+\sqrt{2}\right)(2).$$
$$= \left(10+\sqrt{13}+\sqrt{5}\right)n + 8\sqrt{2} - 30.$$

Hence the result. □

Theorem 4.7. *KG Sombor index of Corona product of complete bipartite graph $K_{m,n}$ with complete graph K_1 is*

$$KG(K_{m,n}\circ K_1) = mn\left(\sqrt{(n+1)^2+(m+n)^2}+\sqrt{(m+1)^2+(m+n)^2}\right)$$
$$+ m\left(\sqrt{(n+1)^2+n^2}+\sqrt{1+n^2}\right) + n\left(\sqrt{(m+1)^2+m^2}+\sqrt{1+m^2}\right).$$

Proof. Let $u_1, u_2, \ldots u_m$ and $v_1, v_2, \ldots v_n$ be the two partitions of vertices of $K_{m,n}$ where $d_{u_i} = n$ and $d_{v_j} = m$; $\forall\ i = 1, 2, \ldots m$ and $j = 1, 2, \ldots n$. The corona product $K_{m,n} \circ K_1$ is obtained by attaching m pendent vertices u_i' to corresponding vertices u_i; $\forall\ \ i = 1, 2, \ldots m$ and n pendent vertices v_j' to corresponding vertices v_j; $\forall\ j = 1, 2, \ldots n$. The KG Sombor Index of Corona product $K_{m,n} \circ K_1$ can be evaluated as below,

$$KG(K_{m,n}\circ K_1) = \sum_{u_iv_j}\left[\sqrt{d_{u_i}^2+d_e^2}+\sqrt{d_{v_j}^2+d_e^2}\right] + \sum_{u_iu_i'}\left[\sqrt{d_{u_i}^2+d_e^2}+\sqrt{d_{u_i'}^2+d_e^2}\right]$$
$$+ \sum_{v_jv_j'}\left[\sqrt{d_{v_j}^2+d_e^2}+\sqrt{d_{v_j'}^2+d_e^2}\right]$$
$$= \sum_{u_iv_j}\left[\sqrt{(n+1)^2+(m+n)^2}+\sqrt{(m+1)^2+(m+n)^2}\right]$$
$$+ \sum_{u_iu_i'}\left[\sqrt{(n+1)^2+n^2}+\sqrt{1+n^2}\right] + \sum_{v_jv_j'}\left[\sqrt{(m+1)^2+m^2}+\sqrt{1+m^2}\right]$$
$$= mn\left(\sqrt{(n+1)^2+(m+n)^2}+\sqrt{(m+1)^2+(m+n)^2}\right)$$
$$+ m\left(\sqrt{(n+1)^2+n^2}+\sqrt{1+n^2}\right) + n\left(\sqrt{(m+1)^2+m^2}+\sqrt{1+m^2}\right).$$

Hence the result. □

5. Concluding Remarks

We derive correlation between dielectric constant and density of hydrocarbons with KG Sombor index. Further, we studied some bounds of KG Sombor index with respect to other indices. We also found KG Sombor index for corona product of certain graphs. The scope of further research extends to the derivation of correlation between different constants of hydrocarbons with various graphical indices.

Acknowledgment

The third author Kajal S. Baldaniya is thankful to the KCG, Education Department, Gujarat State, India for SODH Scholarship reference No. 2023015012.

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