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TOPOLOGICAL ASPECTS ON CORONENE GRAPH USING SOME GRAPH OPERATORS

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Abstract: The Topological index is a numerical parameter of molecular graph which correlates its $QSPR$(Quantitative Structure Property Relationships) and $QSAR$(Quantitative Structure Activity Relationships). In this article, we compute topological indices of some graphs obtained from k-Coronene graph using some graph operations.

Keywords and Phrases: Line graph, semi-total line graph, subdivision graph, semi-total point graph, Topological indices and k-Coronene graph.

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1. Introduction and Preliminaries

Topological indices are the graph invariants which are used to correlate chemical and physical properties of molecular structure. Path number is the first Topological index which is introduced by Harold Wiener (1947) [1], [10], [13], while he was working on Paraffin. So far, various Topological indices have been used in $QSAR/QSPR$ studies. There are some degree based topological indices which are listed beow

The Forgotten index was introduced by B. Furtula [6] and their research collaborators. It is defined

$$F[G] = \sum_{x \in V[G]} deg_G^3 x$$

or

$$F(G) = \sum_{xy \in E(G)} [deg_G^2(x) + deg_G^2(y)].$$

The first Zagreb and second Zagreb indices are introduced by Gutman [7] and their research collaborators. It is defined

$$M_1(G) = \sum_{xy \in E(G)} [deg_G(x) + deg_G(y)]$$

or

$$M_1(G) = \sum_{x \in V(G)} deg_G^2(x)$$

and

$$M_2(G) = \sum_{xy \in E(G)} [deg_G(x).deg_G(y)].$$

The SK index was introduced by R. Kanabur [12] and their research collaborators. It is defined

$$SK(G) = \sum_{xy \in E(G)} \frac{deg_G(x) + deg_G(y)}{2}.$$

The augmented Zagreb index was introduced by B. Furtula [5] and their research collaborators. It is defined

$$AZI(G) = \sum_{xy \in E(G)} \left(\frac{deg_G(x) deg_G(y)}{deg_G(x) + deg_G(y) - 2} \right)^3.$$

The Gourava index was introduced by V. R. Kulli [8] and it is defined as

$$GO_1(G) = \sum_{xy \in E(G)} [deg_G(x) + deg_G(y) + deg_G(x).deg_G(y)].$$

The atom-bond connectivity index was introduced by E. Estrada [3] and their research collaborators. It is defined

$$ABC(G) = \sum_{xy \in E(G)} \sqrt{\frac{deg_G(x) + deg_G(y) - 2}{deg_G(x)deg_G(y)}}$$

The harmonic index was introduced by S. Fajtlowicz [4] and it is defined as

$$H(G) = \sum_{xy \in E(G)} \frac{2}{deg_G(x) + deg_G(y)}$$

The misbalance degree index was introduced by J. Devillers [2] and their research collaborators. It is defined

$$MD(G) = \sum_{xy \in E(G)} |deg_G(x) - deg_G(y)|$$

Definition 1.1. [9] *The* ***line graph*** $L(G)$ *is the graph obtained by associating a vertex with each edge of the graph* G *and two vertices are adjacent with an edge iff the corresponding edges of* G *are adjacent.*

Figure 1: Line graph of P_3

Definition 1.2. [9] *The* ***subdivision graph*** $S(G)$ *is the graph obtained by replacing each of its edge by a path of length 2.*

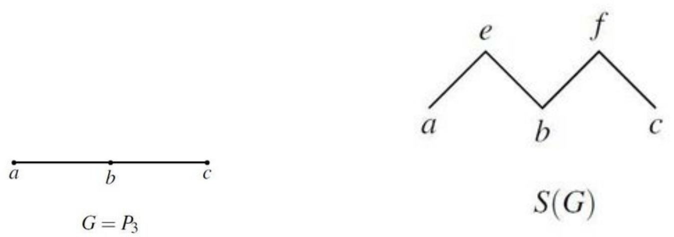

Figure 2: Subdivision graph of P_3

Definition 1.3. [9] *The **semi-total point graph** $R(G)$ is obtained from G by adding a new vertex corresponding to every edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.*

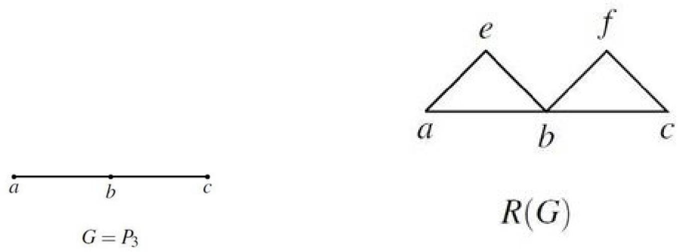

Figure 3: Semi-total point graph of P_3

Coronene: [11] Coronene is very rare mineral carpathite, which occurs naturally and is characterized by fragment of pure coronene rooted in sedimentary rock. $C_{24}H_{12}$ is molecular formula of coronene and is a polycyclic aromatic hydrocarbon (PAH) consisting of around seven benzene rings. The molecular graph of k-coronene ($k = 1, 2, 3, ...$) is shown below.

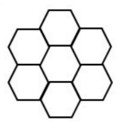

Figure 4: Molecular graph of coronene when $k = 1$

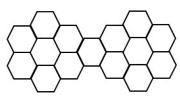

Figure 5: Molecular graph of Dicoronene when $k = 2$

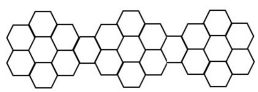

Figure 6: Molecular graph of Tricoronene when $k = 3$

Here i and j are the number of vertices and number of edges in Molecular graph of coronene when $k = 1$.

2. Standard graph operators of Coronene graph

In this section, we study the Topological indices of coronene via graph operators like line graph, subdivision graph, semi-total line graph and semi-total point graph.

Theorem 2.1. *Let ξ be the line graph of k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned} F[\xi] &= 1492k - 352 \\ M_1[\xi] &= 404k - 80. \end{aligned}$$

Proof. Let ξ be a line graph of k-coronene with $kj + 2(k-1)$ vertices and $56k - 8$ edges. In ξ, we have three types of degrees i.e., $2k + 4$ vertices having degree 2, $12k$ vertices having degree 3 and $18k - 6$ vertices having degree 4.
Consider,

$$\begin{aligned} F[G] &= \Sigma_{x \in V[G]} deg_G^3 x \\ F[\xi] &= (2k+4)(2)^3 + 12k(3)^3 + (18k-6)(4)^3 \\ &= 8(2k+4) + 27(12k) + 64(18k-6) \\ &= 16k + 32 + 324k + 1152k - 384 \\ F[\xi] &= 1492k - 352. \end{aligned}$$

A similar method is used to find the value of $M_1[\xi]$.

Theorem 2.2. *Let η be the line graph of subdivision of k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned} F[\eta] &= 1404k + 388 \\ M_1[\eta] &= 496k - 76. \end{aligned}$$

Proof. Let η be a line graph of subdivision of k-coronene with $2kj + 4(k-1)$ vertices and $88k - 10$ edges. In η, we have two types of degrees i.e., $16k + 8$ vertices having degree 2 and $48k - 12$ vertices having degree 3.
Consider,

$$\begin{aligned} F[G] &= \Sigma_{x \in V[G]} deg_G^3 x \\ F[\eta] &= (16k+8)(2)^3 + (48k-12)(3)^3 \\ &= 108k + 64 + 1296k + 324 \\ &= 16k + 32 + 324k + 1152k - 384 \\ F[\eta] &= 1404k + 388. \end{aligned}$$

A similar method is used to find the value of $M_1[\eta]$.

Theorem 2.3. *Let ϑ be the line graph of semi-total point graph of k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned} F[\vartheta] &= 35968k - 7216 \\ M_1[\vartheta] &= 4624k - 760. \end{aligned}$$

Proof. Let ϑ be a line graph of semi-total point graph of k-coronene with $3kj + 6(k-1)$ vertices and $320k - 38$ edges. In ϑ, we have four types of degrees i.e., $16k + 8$ vertices having degree 4, $50k - 8$ vertices having degree 6, $12k$ vertices having degree 8 and $18k - 6$ vertices having degree 10.
Consider,

$$\begin{aligned} F[G] &= \Sigma_{x \in V[G]} deg_G^3 x \\ F[\vartheta] &= (16k+8)(4)^3 + (50k-8)(6)^3 + (12k)(8)^3 + (18k-6)(10)^3 \\ &= 1024k + 512 + 10800k - 728 + 6144k + 18000k - 6000 \\ F[\vartheta] &= 35968k - 7216. \end{aligned}$$

A similar method is used to find the value of $M_1[\vartheta]$.

Theorem 2.4. *Let ρ be the k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned} F[\rho] &= 496k - 76 \\ M_1[\rho] &= 176k - 20 \\ M_2[\rho] &= 242k - 38 \\ SK_1[\rho] &= 88k - 10 \\ AZI[\rho] &= \frac{1}{32}[10145k - 1163] \\ GO_1[\rho] &= 418k - 58 \\ ABC[\rho] &= [12 + 7\sqrt{2}]k + 2\sqrt{2} - 4 \\ H[\rho] &= \frac{59k}{5} \\ MD[\rho] &= 12k. \end{aligned}$$

Proof. Let ρ be a k-coronene with ki vertices and $kj + 2(k-1)$ edges. In ρ, we have three types of edges based on the degree of end vertices of each edge as follows:

(deg_x, deg_y)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$2k+4$	$12k$	$18k-6$

Consider,

$$\begin{aligned}
F[G] &= \Sigma_{xy\in E[G]}[deg_G^2 x + deg_G^2 y] \\
F[\rho] &= (2k+4)(2^2+2^2) + 12k(2^2+3^2) + (18k-6)(3^2+3^2) \\
&= (2k+4)8 + 12k(13) + (18k-6)(18) \\
&= 16k + 32 + 156k + 324k - 108 \\
F[\rho] &= 496k - 76.
\end{aligned}$$

A similar method is used to find the value of $M_1[\rho]$, $M_2[\rho]$, $SK[\rho]$, $AZI[\rho]$, $GO_1[\rho]$, $ABC[\rho]$, $H[\rho]$ and $MD[\rho]$.

Theorem 2.5. *Let ϱ be the subdivision graph of k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned}
F[\varrho] &= 752k - 92 \\
M_1[\varrho] &= 304k - 28 \\
M_2[\varrho] &= 352k - 40 \\
SK_1[\varrho] &= 152k - 14 \\
AZI[\varrho] &= 512k - 32 \\
GO_1[\varrho] &= 656k - 58 \\
ABC[\varrho] &= \frac{1}{\sqrt{2}}[64k - 4] \\
H[\varrho] &= \frac{1}{5}[136k - 4] \\
MD[\varrho] &= 48k - 12.
\end{aligned}$$

Proof. Let ϱ be a subdivision graph of k-coronene with $k(i+j+2)-2$ vertices and $2kj + 4(k-1)$ edges. In ϱ, we have two types of edges based on the degree of end vertices of each edge as follows:

(deg_x, deg_y)	$(2,2)$	$(2,3)$
Number of edges	$16k+8$	$48k-12$

Consider,

$$\begin{aligned} F[G] &= \Sigma_{xy\in E[G]}[deg_G^2 x + deg_G^2 y] \\ F[\varrho] &= (16k+8)(2^2+2^2) + (48k-12)(2^2+3^2) \\ &= (16k+8)8 + (48k-12)13 \\ &= 128k+64+624k-156 \\ F[\varrho] &= 752k-92. \end{aligned}$$

A similar method is used to find the value of $M_1[\varrho]$, $M_2[\varrho]$, $SK[\varrho]$, $AZI[\varrho]$, $GO_1[\varrho]$, $ABC[\varrho]$, $H[\varrho]$ and $MD[\varrho]$.

Theorem 2.6. *Let σ be the semi-total point graph of k-coronene graph for $k = 1, 2, 3, 4, ...$ Then*

$$\begin{aligned} F[\sigma] &= 4224k-624 \\ M_1[\sigma] &= 832k-88 \\ M_2[\sigma] &= 1672k-232 \\ SK_1[\sigma] &= 416k-44 \\ AZI[\sigma] &= \frac{1}{3375}[5783852k-796784] \\ GO_1[\sigma] &= 2504k-224 \\ ABC[\sigma] &= \frac{1}{\sqrt{2}}[64k-4] + \sqrt{\frac{3}{8}}[2k+4] + \frac{12k}{\sqrt{3}} + \sqrt{\frac{5}{13}}[18k-6] \\ H[\sigma] &= \frac{697k}{30} - \frac{1}{3} \\ MD[\sigma] &= 248k-8. \end{aligned}$$

Proof. Let σ be a semi-total point graph of k-coronene with $k(i+j+2)-2$ vertices and $3kj+6(k-1)$ edges. In σ, we have five types of edges based on the degree of end vertices of each edge as follows:

(deg_x, deg_y)	$(2,4)$	$(2,6)$	$(4,4)$	$(4,6)$	$(6,6)$
Number of edges	$16k+8$	$48k-12$	$2k+4$	$12k$	$18k-6$

Consider,

$$\begin{aligned} F[G] &= \Sigma_{xy\in E[G]}[deg_G^2 x + deg_G^2 y] \\ F[\sigma] &= (16k+8)(2^2+4^2)+(48k-12)(2^2+6^2)+(2k+4)(4^2+4^2) \\ &+ 12k(4^2+6^2)+(18k-6)(6^2+6^2) \\ &= (16k+8)20+(48k-12)40+(2k+4)32+12k(52)+(18k-6)72 \\ F[\sigma] &= 422k-624. \end{aligned}$$

A similar method is used to find the value of $M_1[\sigma]$, $M_2[\sigma]$, $SK[\sigma]$, $AZI[\sigma]$, $GO_1[\sigma]$, $ABC[\sigma]$, $H[\sigma]$ and $MD[\sigma]$.

3. Conclusion

In this work, we study few Topological indices of k-coronene graph using graph operators such as line graph, subdivision graph, semi-total point graph. These results are useful to study the quantitative structure property relation and quantitative structure activity relation of k-coronene graph.

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