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# On Topological Properties Of Dyck-56 Networks

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**Abstract**

In $QSAR/QSPR$ study, physico-chemical properties and topological indices such as Randić, atom-bond connectivity $(ABC)$ and geometric-arithmetic $(GA)$ index are used to predict the bioactivity of chemical compounds. A topological index can be considered as a transformation of a chemical structure into a real number, these topological descriptors significantly correlate certain physico-chemical properties of the corresponding chemical compounds. Graph theory has found a considerable use in this area of research. In this paper, we derive analytical closed results for the general Randić index $R_\alpha(G)$ (for different values of $\alpha$), first Zagreb, $ABC$ and $GA$ indices for the Dyck-56 chemical networks for the first time.

**Key words:** General Randić index, $ABC$ index, $GA$ index, Dyck-56 network

**2010 Mathematics Subject Classification** : 05C12, 05C90

## 1 Introduction

In theoretical chemistry, the graph theoretic models can be used to study the properties of molecules. Topological indices plays a vital role in QSAR/QSPR study. The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in QSAR/QSPR researches [1, 5, 7, 8, 9, 12, 13, 14, 16, 17, 18, 20, 21, 22, 23, 33, 35, 4, 24, 25]. In the last few years, the number of proposed molecular descriptors is rapidly growing, they correlate the certain physico-chemical properties of chemical compounds. A close correlation of Randić index to the boiling point and Kovats constants has been found. A good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes is provided by the atom-bond connectivity $(ABC)$ index. For certain

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physico-chemical properties like boiling point, Entropy, Enthalpy of vaporization, standard Enthalpy of vaporization, Enthalpy of formation and acentric factor, the predictive power of $GA$ index is better than the predictive power of the Randić connectivity index [6]. The topological properties of certain networks were studied recently by M Imran et al.[26, 27, 28, 29, 30, 31]. In this paper we compute these indices for Dyck-$56$ network $(Figs.1, 2, 3)$ [32, 2].

Let $G$ be a connected graph with $n$ vertices and $m$ edges. Let $V(G)$ and $E(G)$ be its vertex and edge sets, respectively. A *network* is simply a connected graph having no multiple edges and loops. A *chemical graph* is a graph whose vertices denotes atoms and edges denotes bonds between the atoms and any underlying chemical structure. The *degree* of a vertex $u$ in a graph $G$ is the number of edges joining to $u$ and is denoted by $d_u$. In a chemical graph the degree of any vertex is at most $4$ [15]. The *distance* between the vertex $u$ and $v$ is the length of the shortest path joining $u$ and $v$ and is denoted by $d_G(u, v)$ [11].

One of the oldest degree based topological index is Randić index [34] and is defined as,

$$R_{-\frac{1}{2}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u \times d_v)}}.$$

The general Randić index [3] $R_\alpha(G)$ is defined as,

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u \times d_v)^\alpha.$$

The first Zagreb indices of a graph $G$ is defined as [19],

$$M_1(G) = \sum_{uv \in E(G)} [d_u + d_v].$$

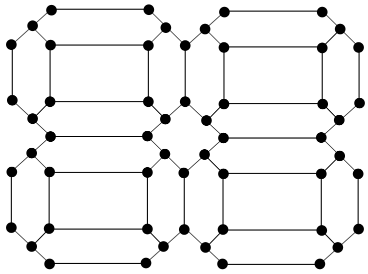
A well-known degree based topological index is atom-bond connectivity $ABC$ index introduced by Estrada et al. in [10] and defined as,

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Another well-known topological index is geometric-arithmetic $(GA)$ index [36] and is defined as,

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

## 2 Results for Dyck-56 networks



$Fig.1 : Dyck - 56_{2\times2}(A)$ network

| Table 1: Edge partition of Dyck-56 (A) network | |
|---|---|
| $(d_u, d_v)$, where $uv \in E(G)$ | Number of edges |
| $(2,2)$ | $4n$ |
| $(2,3)$ | $8n$ |
| $(3,3)$ | $18n^2 - 10n$ |

**Theorem 2.1.** Let $G$ be the $Dyck - 56_{n\times n}$(A) network, then its general Randic index is equal to

$$R_\alpha(G) = \begin{cases} 162n^2 - 26n & \text{if } \alpha = 1; \\ 54n^2 + 8n\sqrt{6} - 22n & \text{if } \alpha = \frac{1}{2}; \\ \frac{1}{9}[18n^2 + 11n] & \text{if } \alpha = -1; \\ n\left[\frac{2\sqrt{6}+8}{\sqrt{6}} + \frac{18n-10}{3}\right] & \text{if } \alpha = \frac{-1}{2}; \end{cases}$$

**Proof:** The number of vertices and edges in $G$ are $12n^2 + 4n$ and $18n^2 - 2n$ respectively. There are three types of edges in $G$, based on degrees of end vertices of each edge. Table 1, shows the edge partitions of $G$.

By using edge partition given in table 1, we get

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u \times d_v)^\alpha$$

For $\alpha = 1$,

$$\begin{aligned}
R_1(G) &= \sum_{uv \in E(G)} (d_u \times d_v) \\
&= 4n(2 \times 2) + 8n(2 \times 3) + (18n^2 - 10n)(3 \times 3) \\
&= 162n^2 - 26n.
\end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= \sum_{uv \in E(G)} \sqrt{(d_u \times d_v)} \\
&= 4n\sqrt{(2 \times 2)} + 8n\sqrt{(2 \times 3)} + (18n^2 - 10n)\sqrt{(3 \times 3)} \\
&= 54n^2 + 8n\sqrt{6} - 22n.
\end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned}
R_{-1}(G) &= \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)} \\
&= 4n\frac{1}{(2 \times 2)} + 8n\frac{1}{(2 \times 3)} + (18n^2 - 10n)\frac{1}{(3 \times 3)} \\
&= \frac{1}{9}[18n^2 + 11n].
\end{aligned}$$

For $\alpha = -\frac{1}{2}$,

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u \times d_v)}} \\
&= 4n\frac{1}{\sqrt{(2 \times 2)}} + 8n\frac{1}{\sqrt{(2 \times 3)}} + (18n^2 - 10n)\frac{1}{\sqrt{(3 \times 3)}} \\
&= n\left[\frac{2\sqrt{6} + 8}{\sqrt{6}} + \frac{18n - 10}{3}\right].
\end{aligned}$$

■

**Theorem 2.2.** Let $G$ be the $Dyck-56_{n\times n}$(A) network, then its first Zagreb index is equal to

$$M_1(G) = 108n^2 - 4n.$$

**Proof:** By using edge partition from table 1, the result follows.

$$\begin{aligned} M_1(G) &= \sum_{uv\in E(G)} (d_u + d_v) \\ &= 4n(2+2) + 8n(2+3) + (18n^2 - 10n)(3+3) \\ &= 108n^2 - 4n. \end{aligned}$$

∎

**Theorem 2.3.** Let $G$ be the $Dyck-56_{n\times n}$(A) network, then its $ABC$ index is equal to

$$ABC(G) = 12n^2 + \frac{n}{3}(18\sqrt{2} - 20).$$

**Proof:** By using edge partition from table 1, the result follows.

$$\begin{aligned} ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 4n\sqrt{\frac{2+2-2}{4}} + 8n\sqrt{\frac{2+3-2}{6}} + (18n^2 - 10n)\sqrt{\frac{3+3-2}{9}} \\ &= 12n^2 + \frac{n}{3}(18\sqrt{2} - 20). \end{aligned}$$

∎

**Theorem 2.4.** Let $G$ be the $Dyck-56_{n\times n}$(A) network, then its $GA$ index is equal to

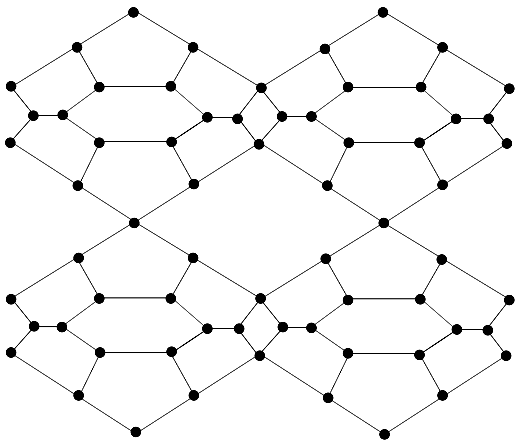
$$GA(G) = 18n^2 - 6n + \frac{16\sqrt{6}n}{5}.$$

**Proof:** By using edge partition from table 1, the result follows.

$$GA(G) = \sum_{uv\in E(G)} 2\frac{\sqrt{d_u d_v}}{d_u + d_v}$$

$$= 4n\left(2\frac{\sqrt{2\times 2}}{2+2}\right) + 8n\left(2\frac{\sqrt{2\times 3}}{2+3}\right) + (18n^2 - 10n)\left(2\frac{\sqrt{3\times 3}}{3+3}\right)$$
$$= 18n^2 - 6n + \frac{16\sqrt{6}n}{5}.$$

∎



$Fig.2 : Dyck - 56_{2\times 2}(B)$ network

| Table 2: Edge partition of Dyck-56 (B) network | |
|---|---|
| $(d_u, d_v)$, where $uv \in E(G)$ | Number of edges |
| $(2,3)$<br>$(3,3)$<br>$(3,4)$ | $8(n+1)$<br>$12n^2$<br>$12n(n-1)$ |

**Theorem 2.5.** Let $G$ be the $Dyck-56_{n\times n}$(B) network, then its general Randic index is equal to

$$R_\alpha(G) = \begin{cases} 252n^2 - 96n + 48 & \text{if } \alpha = 1; \\ 36n^2 + 8\sqrt{6}(n+1) + 24\sqrt{3}n(n-1) & \text{if } \alpha = \frac{1}{2}; \\ \frac{7n^2+n+4}{3} & \text{if } \alpha = -1; \\ 4n^2 + 2\sqrt{3}n(n-1) + \frac{8(n+1)}{\sqrt{6}} & \text{if } \alpha = \frac{-1}{2}; \end{cases}$$

**Proof:** The number of vertices and edges in $G$ are $18n^2 - 3n$ and $24n^2 - 4n + 8$ respectively. There are three types of edges in $G$, based on degrees of end vertices of each edge. Table 2 shows the edge partitions of $G$.
By using edge partition given in table 2, we get

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u \times d_v)^\alpha$$

For $\alpha = 1$,

$$\begin{aligned} R_1(G) &= \sum_{uv\in E(G)} (d_u \times d_v) \\ &= 8(n+1)(2\times 3) + 12n^2(3\times 3) + 12n(n-1)(3\times 4) \\ &= 252n^2 - 96n + 48. \end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{uv\in E(G)} \sqrt{(d_u \times d_v)} \\ &= 8(n+1)\sqrt{6} + 12n^2\sqrt{9} + 12n(n-1)\sqrt{12} \\ &= 36n^2 + 8\sqrt{6}(n+1) + 24\sqrt{3}n(n-1). \end{aligned}$$

For $\alpha = -1$,

$$
\begin{aligned}
R_{-1}(G) &= \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)} \\
&= \frac{8(n+1)}{6} + \frac{12n^2}{9} + \frac{12n(n-1)}{12} \\
&= \frac{7n^2+n+4}{3}.
\end{aligned}
$$

For $\alpha = -\frac{1}{2}$,

$$
\begin{aligned}
R_{\frac{-1}{2}}(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u \times d_v)}} \\
&= \frac{8(n+1)}{\sqrt{6}} + \frac{12n^2}{\sqrt{9}} + \frac{12n(n-1)}{\sqrt{12}} \\
&= 4n^2 + 2\sqrt{3}n(n-1) + \frac{8(n+1)}{\sqrt{6}}.
\end{aligned}
$$

∎

**Theorem 2.6.** Let $G$ be the $Dyck - 56_{n\times n}$(B) network, then its first Zagreb index is equal to $M_1(G) = 156n^2 - 44n + 40$.

**Proof:** By using edge partition from table 2, the result follows.

$$
\begin{aligned}
M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v) \\
&= 8(n+1)(2+3) + 12n^2(3+3) + 12n(n-1)(3+4) \\
&= 156n^2 - 44n + 40.
\end{aligned}
$$

∎

**Theorem 2.7.** Let $G$ be the $Dyck - 56_{n\times n}$(B) network, then its $ABC$ index is equal to $ABC(G) = 8n^2 + 4\sqrt{2}(n+1) + 2\sqrt{15}n(n-1)$.

**Proof:** By using edge partition from table 2, the result follows.

$$\begin{aligned}
ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\
&= 8(n+1)\sqrt{\frac{2+3-2}{6}} + 12n^2\sqrt{\frac{3+3-2}{9}} + 12n(n-1)\sqrt{\frac{3+4-2}{12}} \\
&= 8n^2 + 4\sqrt{2}(n+1) + 2\sqrt{15}n(n-1).
\end{aligned}$$

∎

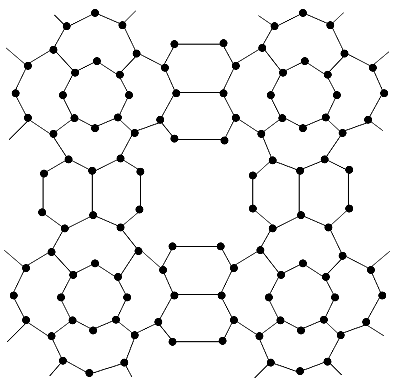
**Theorem 2.8.** Let $G$ be the $Dyck - 56_{n\times n}$(B) network, then its $GA$ index is equal to

$$GA(G) = 12n^2 + \frac{16\sqrt{6}}{5}(n+1) + \frac{48\sqrt{3}}{7}(n(n-1)).$$

**Proof:** By using edge partition from table 2, the result follows.

$$\begin{aligned}
GA(G) &= \sum_{uv \in E(G)} 2\frac{\sqrt{d_u d_v}}{d_u + d_v} \\
&= 8(n+1)\left(2\frac{\sqrt{6}}{5}\right) + 12n^2\left(2\frac{\sqrt{9}}{6}\right) + (12n(n-1))\left(2\frac{\sqrt{12}}{7}\right) \\
&= 12n^2 + \frac{16\sqrt{6}}{5}(n+1) + \frac{48\sqrt{3}}{7}(n(n-1)).
\end{aligned}$$

∎



$Fig.3 : Dyck - 56_{2\times 2}(C)$ network

| Table 3: Edge partition of Dyck-56 (C) network | |
|---|---|
| $(d_u, d_v)$, where $uv \in E(G)$ | Number of edges |
| $(2,3)$ | $16n^2$ |
| $(3,3)$ | $22n^2 - 10n$ |
| $(2,2)$ | $4n(n-1)$ |

**Theorem 2.9.** Let $G$ be the $Dyck - 56_{n\times n}$(C) network, then its general Randic index is equal to

$$R_\alpha(G) = \begin{cases} 310n^2 - 106n & \text{if } \alpha = 1; \\ (16\sqrt{6} + 74)n^2 - 30n - 8 & \text{if } \alpha = \frac{1}{2}; \\ \frac{55n^2 - 19n}{9} & \text{if } \alpha = -1; \\ \frac{16n^2}{\sqrt{6}} + \frac{22n^2 - 10n}{3} + 2n(n-1) & \text{if } \alpha = \frac{-1}{2}; \end{cases}$$

**Proof:** The number of vertices and edges in $G$ are $32n^2 - 8n$ and $42n^2 - 14n$ respectively. There are three types of edges in $G$, based on degrees of end vertices of each edge. Table 3 shows the edge partitions of $G$. By using edge partition given in Table 3, we get

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u \times d_v)^\alpha$$

For $\alpha = 1$,

$$\begin{aligned} R_1(G) &= \sum_{uv\in E(G)} (d_u \times d_v) \\ &= 16n^2(6) + (22n^2 - 10n)(9) + 4n(n-1)(4) \\ &= 310n^2 - 106n. \end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{uv\in E(G)} \sqrt{(d_u \times d_v)} \\ &= 16n^2\sqrt{6} + (22n^2 - 10n)\sqrt{9} + 4n(n-1)\sqrt{4} \end{aligned}$$

$$= (16\sqrt{6} + 74)n^2 - 30n - 8.$$

For $\alpha = -1$,

$$\begin{aligned} R_{-1}(G) &= \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)} \\ &= \frac{16n^2}{6} + \frac{22n^2 - 10n}{9} + \frac{4n^2 - 4n}{4} \\ &= \frac{55n^2 - 19n}{9}. \end{aligned}$$

For $\alpha = -\frac{1}{2}$,

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u \times d_v)}} \\ &= \frac{16n^2}{\sqrt{6}} + \frac{22n^2 - 10n}{\sqrt{9}} + \frac{4n^2 - 4n}{\sqrt{4}} \\ &= \frac{16n^2}{\sqrt{6}} + \frac{22n^2 - 10n}{3} + 2n(n-1). \end{aligned}$$

∎

**Theorem 2.10.** Let $G$ be the $Dyck - 56_{n \times n}$(C) network, then its first Zagreb index is equal to

$$M_1(G) = 228n^2 - 76n.$$

**Proof:** By using edge partition from Table 3, the result follows.

$$\begin{aligned} M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v) \\ &= 16n^2(2+3) + (22n^2 - 10n)(3+3) + 4n(n-1)(2+2) \\ &= 228n^2 - 76n. \end{aligned}$$

∎

**Theorem 2.11.** Let $G$ be the $Dyck - 56_{n \times n}$(C) network, then its $ABC$ index is equal to

$$ABC(G) = \left(\frac{24\sqrt{2}+44}{3}\right)n^2 + 2\sqrt{2}(n(n-1)) - \frac{20}{3}n.$$

**Proof:** By using edge partition from Table 3, the result follows.

$$\begin{aligned}
ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\
&= 16n^2\sqrt{\frac{2+3-2}{6}} + (22n^2-10n)\sqrt{\frac{3+3-2}{9}} + 4n(n-1)\sqrt{\frac{2+2-2}{4}} \\
&= \left(\frac{24\sqrt{2}+44}{3}\right)n^2 + 2\sqrt{2}(n(n-1)) - \frac{20}{3}n.
\end{aligned}$$

∎

**Theorem 2.12.** Let $G$ be the $Dyck-56_{n\times n}$(C) network, then its $GA$ index is equal to

$$GA(G) = \left(\frac{32\sqrt{6}+130}{5}\right)n^2 - 14n.$$

**Proof:** By using edge partition from Table 3, the result follows.

$$\begin{aligned}
GA(G) &= \sum_{uv\in E(G)} 2\frac{\sqrt{d_u d_v}}{d_u+d_v} \\
&= 16n^2\left(2\frac{\sqrt{6}}{5}\right) + (22n^2-10n)\left(2\frac{\sqrt{9}}{6}\right) + (4n(n-1))\left(2\frac{\sqrt{4}}{4}\right) \\
&= \left(\frac{32\sqrt{6}+130}{5}\right)n^2 - 14n.
\end{aligned}$$

∎

## 3 Conclusion

In this paper, certain degree based topological indices, namely general Randić index, $ABC$, $GA$ and first Zagreb index for Dyck-56 network were studied for the first time and analytical closed formulas for this network were determined, which will help experts working in network science understand and explore the underlying topologies of these networks. To construct and study new architectures has always been an open problem in both network and art/design sciences.

In future, we are interested to design some new architectures/networks and then study their toplogical indices which will be helpful to understand their underlying topologies.

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