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The Wiener index of some algebraic graphs and some applications

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Abstract

In mathematical chemistry, we periodically use the graphs. In particular, the vertex in G is refers to the atom in a molecule, and the edge is refers to the bonds. The main object is to study the characteristics of model's graph. In our work, we discuss the Wiener index of some algebraic graph (Cayley graph and Dihedral Graph). Moreover, we have given a particular example of Wiener index for the structure of tecovirimat and the structure of cidofovir. Finally, the relationship between the Wiener index BO and boiling point *WI* is found for the data is approximated by $BO = 181(WI)^{0.1775}$, where the boiling point of a family of hydrocarbons, by using model's graph of the molecules.

Subject Classification (2010): *05C09, 05C25.*

Keywords: *Wiener index, Cayley graph, Dihedral graph.*

1. Introduction

To delve into mathematical chemistry well, it is essential to understand graph theory. It uses graphs to create mathematical models to study chemical properties and reactions, which helps in the development of chemistry[6]. Molecular compounds are graph models. In mathematical chemistry, topological indices are numbers that encode the structural properties of compounds[7]. Researchers first used topological indices in 1947 in chemistry and biology sciences, when the Wiener index was discovered to explain the relationship between the chemical and physical properties of organic compounds through molecular graphs [8].

The following equality is the definition of Wiener index, it was the first topological index, and it introduced by Wiener in 1947 [8]. $WI(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)$, where $d(u,v)$ is the distance between g and h. He found the important relationship, it is between Wiener index WI and boiling point BO for the data which is approximated by $BO = 181(WI)^{0.1775}$, In this paper, we studied the Wiener index, it depends on the distance between the vertices. We presented the all different between standard graph Γ and common neighbourhood graph $\mathbf{Con}(\Gamma)$ about the number of edges. Moreover, we gave new examples for this topological index for some chemical structures. Finally, we studied the relationship $BO = 181(WI)^{0.1775}$, for these chemical structures. In this paper, all graphs considered are finite, connected, and simple graphs. Let G be a connected graph of order n, it is the number of vertices in the set of vertices V. Suppose that $g, h \in V$, we denote $d(g,h)$ for the distance between g and h in G, which is the length of shortest path between g and h [1]. In G, the degree of $w \in V$ is denoted by $d(w)$ [2]. For $F \subset V$, the subgraph of G induced by F is denoted by $< F >$. The cycle and the path on n vertices were denoted by C_n and P_n, respectively. You can find the definitions and notation, which are not presented here in [4, 5] and [12-17]. The set of edges of G is denoted by E. A topological index is a number that can be extracted from the concepts of a graph, which does not change if the drawing of graph changes, while the two graph are isomorphic. A topological index that is calculated using the distances between vertices is called a "distance index topological index". Salah and Shelash [12], introduced the structure graphs for some of finite group from using Cayley graph definition. Shuker and Shelash [11], presented the one of important application in graph theory with name Pseudospectrum Energy of Graphs for some of finite group. For more information, see references [3, 9, 10, 18-21],

2. Auxiliary results

Definition 1: [12] Let us fixed a positive integer $n \neq 3$, The set of certain non-abelain group of order $2n$ is called the Dihedral group, it is denoted by D_{2n}. It is generated by a and b, s.t., a rotation a of order n, and reflection b of order 2. We can write the $2n$ elements of D_{2n} as the following: $\{1, a, a^2, \cdots, a^{n-2}, a^{n-1}, b, ab, a^2b, \cdots, a^{n-2}b, a^{n-1}b\}$

Lemma 2: [12*] The computing of the Cayley graph of Cyclic groups can be given in the following statements:*

$$Cay(C_n, F) = \begin{cases} C_n & F = F_1 \\ K_4 & F = F_2, F_3, n = 4 \\ M_{\frac{n}{2}} & F = F_2, n \geq 6 \\ GP(\frac{n}{2}, 1) & F = F_3, 2 \nmid \frac{n}{2} \\ M_{\frac{n}{2}} & F = F_3, 2 | \frac{n}{2} \end{cases}$$

Where $F_1 = \{a, a^{-1}\}$, $F_2 = \{a, a^{-1}, a^{\frac{n}{2}}\}$, $F_3 = \{a^{\frac{n}{2}+1}, a^{\frac{n}{2}-1}, a^{\frac{n}{2}}\}$, $F_4 = \{a, a^{-1}\}, F_5 = \{a, a^{-1}, b\}, F_6 = \{ab, a^{-1}b, b\}$. Also, the Dihedral Group of some graphs are computed in the following simple form:

$$Cay(D_{2n}, F) = \begin{cases} K_2 \cup K_2 & F = F_4, n = 2 \\ C_n \cup C_n & F = F_4, n \geq 3 \\ C_4 & F = F_5, F_6, n = 2 \\ GP(n, 1) & F = F_5, n \geq 3 \\ M_n & F = F_6, 2 \nmid n \geq 3 \\ GP(n, 1) & F = F_6, 2 | n \geq 4 \end{cases}$$

Theorem 3: [12] *The statements below are valid:*

- $Cay(C_n, F_1) \times Cay(C_2, F_1) = \begin{cases} C_{2n} & 2 \nmid n \\ C_n \cup C_n & 2 | n \end{cases}.$
- $Cay(C_n, F_1) \boxdot Cay(C_2, F_1) = GP(n, 1)$
- $Cay(C_n, F_1) \boxtimes Cay(C_2, F_1) = \begin{cases} K_{2n} & n = 2,3 \\ QW_n & n \geq 4 \end{cases}.$

- $$Cay(C_n, F_2) \times Cay(C_2, F_1) = \begin{cases} GP(n,1) & 2 \mid \frac{n}{2} \\ M_{(\frac{n}{2})} \cup M_{(\frac{n}{2})} & 2 \nmid \frac{n}{2} \end{cases}.$$
- $Cay(C_n, F_2) \boxtimes Cay(C_2, F_1) = K_8\ , n = 4$
- $Cay(C_n, F_3) \times Cay(C_2, F_1) = GP(n, 1);$
- $Cay(C_n, F_3) \boxtimes Cay(C_2, F_1) = K_8\ n = 4.$

3. The Wiener index for some standard of graph

Lemma 4: *The following statements are holds:*

- If $\Gamma = C_n$, then $E(\Gamma) = n$, and the Wiener is: $WI(\Gamma) = \begin{cases} \frac{n^3}{8} & 2 \nmid n \\ \frac{n(n-1)(n+1)}{8} & 2 \nmid n \end{cases}$.
- If $\Gamma = K_n$, then $E(\Gamma) = n(n-1)$, and the Wiener is: $WI(\Gamma) = \frac{n(n-1)}{2}$
- If $\Gamma = P_n$, then $E(\Gamma) = (n-1)$, and the Wiener is: $WI(\Gamma) = \frac{n(n^2-1)}{6}$
- If $\Gamma = GP(n, 1)$, then $E(\Gamma) = 3n$, and the Wiener is: $WI(\Gamma) = \frac{n^2(n+2)}{2}$
- If $\Gamma = M(n)$, then $E(\Gamma) = 3n$, and the Wiener is: $WI(\Gamma) = \frac{n}{4}[2n(n+2) - 3 - (-1)^n]$
- If $\Gamma = QW(n)$, then $E(\Gamma) = 4n$, and the Wiener is: $WI(\Gamma) = \frac{n}{4}[2n(n+2) - 3 - (-1)^n]$

Proposition 5: The Wiener indices of the Cayley graph of cyclic groups, when $F_1 = \{a, a^{-1}\}$, $F_2 = \{a, a^{-1}, a^{\frac{n}{2}}\}$, and $F_3 = \{a^{\frac{n}{2}+1}, a^{\frac{n}{2}-1}, a^{\frac{n}{2}}\}$ are computed below with a clearly form:

$$WI(Cay(C_n, F)) = \begin{cases} WI(C_n) & F = F_1 \\ WI(K_4) & F = F_2, n = 4 \\ WI(M_n) & F = F_2, n \geq 6 \\ WI(K_4) & F = F_3, n = 4 \\ WI(GP(\frac{n}{2}, 1)) & F = F_3, 2 \nmid \frac{n}{2} \\ WI(M_n) & F = F_3, 2 \mid \frac{n}{2} \end{cases}.$$

Proposition 6: The Wiener indices of D_{2n}, whose the set of finite elements are $F_1 = \{a, a^{-1}\}, F_2 = \{a, a^{-1}, b\}, F_3 = \{ab, a^{-1}b, b\}, F_4 = \{a, a^{-1}, a^{\frac{n}{2}}\}, F_5 = \{a^{\frac{n}{2}+1}, a^{\frac{n}{2}-1}, a^{(}n/2)\}$, and $F_6 = \{a, a^{-1}, b, ab, a^{-1}b\}$, is given in the following:

$$WI(Cay(D_{2n},F)) = \begin{cases} WI(K_2 \cup K_2) & F = F_1, n = 2 \\ WI(C_n \cup C_n) & F = F_1, n \geq 2 \\ WI(C_4) & F = F_2, n = 2 \\ WI(GP(n,1)) & F = F_2, n \geq 3 \\ WI(C_4) & F = F_3, n \geq 2 \\ WI(M_n) & F = F_3, 2 \nmid n \\ WI(GP(n,1)) & F = F_3, 2|n \\ WI(K_4 \cup K_4) & F = F_4, n = 4 \\ WI(M(\frac{n}{2}) \cup M(\frac{n}{2})) & F = F_4, n \geq 6 \\ WI(K_4 \cup K_4) & F = F_5, n = 4 \\ WI(M(\frac{n}{2}) \cup M(\frac{n}{2})) & F = F_5, 2|n \\ WI(GP(\frac{n}{2}) \cup GP(\frac{n}{2})) & F = F_5, 2 \nmid n \\ WI(K_2n) & F = F_6, n = 2,3 \\ WI(QW_n) & F = F_6, 2 \geq 4 \end{cases}.$$

Theorem 7: *The following statements are holds:*

- $$WI(Cay(C_n,F_1) \times Cay(C_2,F_1)) = \begin{cases} WI(C_{2n}) & 2 \nmid n \\ WI(C_n \cup C_n) & 2|n \end{cases}.$$
- $$WI(Cay(C_n,F_1) \boxdot Cay(C_2,F_1)) = WI(GP(n,1))$$
- $$WI(Cay(C_n,F_1) \boxtimes Cay(C_2,F_1)) = \begin{cases} WI(K_{2n}) & n = 2,3 \\ WI(QW_n) & n \geq 4 \end{cases}.$$

4. Applications of some Chemical Structure

In this section, we will calculate Wiener index, for some Chemical Structure.

Example 8: Let G be the structure of cidofovir ($C_8H_{14}N_3O_6P_1$), see Figure 1. The Wiener index of G is: $WI(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = 665$, where the vertices u and v represent the vertices C_i $(1 \leq i \leq 8)$, N_j $(1 \leq j \leq 3)$, O_k $(1 \leq k \leq 6)$, and P_1.

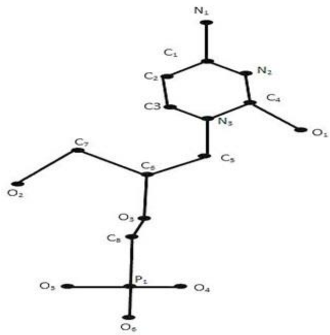

Figure 1

The structure of Cidofovir C_8H_14N_3O_6P_1

$$\begin{bmatrix}
0 & 1 & 2 & 2 & 3 & 3 & 4 & 4 & 5 & 6 & 7 & 8 & 7 & 8 & 9 & 10 & 10 & 10 \\
1 & 0 & 1 & 1 & 2 & 2 & 3 & 3 & 4 & 5 & 6 & 7 & 6 & 7 & 8 & 9 & 9 & 9 \\
2 & 1 & 0 & 2 & 1 & 3 & 2 & 4 & 3 & 4 & 5 & 6 & 5 & 6 & 7 & 8 & 8 & 8 \\
2 & 1 & 2 & 0 & 3 & 1 & 2 & 2 & 3 & 4 & 5 & 6 & 5 & 6 & 7 & 8 & 8 & 8 \\
3 & 2 & 1 & 3 & 0 & 2 & 1 & 3 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 7 & 7 \\
3 & 2 & 3 & 1 & 2 & 0 & 1 & 1 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 7 & 7 \\
4 & 3 & 2 & 2 & 1 & 1 & 0 & 2 & 1 & 2 & 3 & 4 & 3 & 4 & 5 & 6 & 6 & 6 \\
4 & 3 & 4 & 2 & 3 & 1 & 2 & 0 & 3 & 4 & 5 & 6 & 5 & 6 & 7 & 8 & 8 & 8 \\
5 & 4 & 3 & 3 & 2 & 2 & 1 & 3 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 5 & 5 \\
6 & 5 & 4 & 4 & 3 & 3 & 2 & 4 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 4 & 4 & 4 \\
7 & 6 & 5 & 5 & 4 & 4 & 3 & 5 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 5 & 5 \\
8 & 7 & 6 & 6 & 5 & 5 & 4 & 6 & 3 & 2 & 1 & 0 & 3 & 4 & 5 & 6 & 6 & 6 \\
7 & 6 & 5 & 5 & 4 & 4 & 3 & 5 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 3 & 3 \\
8 & 7 & 6 & 6 & 5 & 5 & 4 & 6 & 3 & 2 & 3 & 4 & 1 & 0 & 1 & 2 & 2 & 2 \\
9 & 8 & 7 & 7 & 6 & 6 & 5 & 7 & 4 & 3 & 4 & 5 & 2 & 1 & 0 & 1 & 1 & 1 \\
10 & 9 & 8 & 8 & 7 & 7 & 6 & 8 & 5 & 4 & 5 & 6 & 3 & 2 & 1 & 0 & 2 & 2 \\
10 & 9 & 8 & 8 & 7 & 7 & 6 & 8 & 5 & 4 & 5 & 6 & 3 & 2 & 1 & 2 & 0 & 2 \\
10 & 9 & 8 & 8 & 7 & 7 & 6 & 8 & 5 & 4 & 5 & 6 & 3 & 2 & 1 & 2 & 2 & 0
\end{bmatrix}$$

Figure 2

The distance matrix

We solve this structure using another solution, the method based on the figure 2. The distance matrixsuch that, $WI(G) = 1/2 \sum_{v \in V(G)} t_G(v)$, where $t_G(v)$ of a vertex $v \in V(G)$ is the sum of distances between v and all other vertices of G, see the distance matrix. We found the same result: $WI(G) = 1330/2 = 665$. So, the expected boiling point will be: $B = 181(665)^{0.1775} = 573.7588757559$.

Example 9: Let G be the structure of tecovirimat $(C_{19}H_{15}F_3N_2O_3)$, see Figure 3, then $WI(G)$ is: $WI(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) = 1878$, where the vertices u and v represent the vertices C_a $(1 \le a \le 19)$, F_b $(1 \le b \le 3)$, N_c $(1 \le c \le 2)$, and O_e $(1 \le e \le 3)$. So the expected boiling point will be:

$$B = 181(1878)^{0.1775} = 689.8577406576.$$

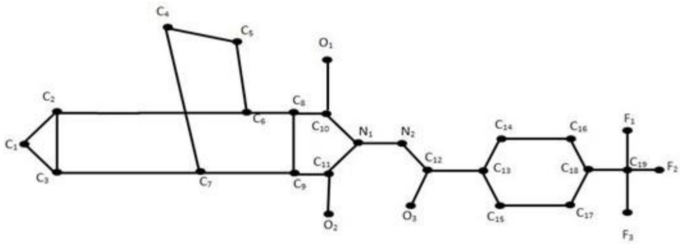

Figure 3
Structure of tecovirimat ($C_{19}H_{15}F_3N_2O_3$).

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