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ZAGREB INDICES FOR CHAINS OF IDENTICAL HEXAGONAL CYCLES

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Abstract The number of edges incident with a vertex v is called a *degree* of a vertex v. Given the importance of the degrees of vertices for chemical applications, which correspond to the number of bonds that fall on atoms, our interest was in finding formulas of indices that depend on the degrees of vertices, such as: first Zagreb, second Zagreb, complement first Zagreb and complement second Zagreb indices. We found an iterative and general formulas for these indices that depend on the previous cycles or on the number of cycles for graphs construct from identical edges the hexagonal cycles and we give some examples for chemical applications in this article.

1 Introduction

The *degree* of a vertex v is the number of edges incident with v where v is a vertex belong to a vertex set $V(G)$ of a connected graph G and denoted by deg v; a vertex of degree one is an *end vertex*, or *pendant* of G. A vertex of degree 0 is *isolated.* In this article, we consider the graph G is a simple, connected and undirected graph. An *invariant* of a graph G is a number associated with G which has the same value for any graph isomorphic to G, for known a lot of basic concepts about graph theory, see [1]. The order and size of a graph are two simple graph invariants. And there are many indices such as: Wiener index [2], Schultz and modified Schultz indices [3], $D-$ index [4], M_n-index [5] and detour number [6], that are *invariant*s for isomorphic graphs, which have many applications, especially in chemistry [7-9].

The first Zagreb index $Z1(G)$ was first time considered in 1972, [10] but the second Zagreb index $Z2(G)$ was first time considered in 1975, [11] of a connected graph G and were defined as follows:

$$Z1(G) = \sum_{uv\in E(G)} (degu + degv),$$

$$Z2(G) = \sum_{uv\in E(G)} (degu \times degv).$$

From above definitions, we note that the Zagreb indices can be viewed as the contributions of pairs of adjacent vertices. But there are another indices contrary to the adjacent condition (non-adjacent pairs of vertices), this is known coindices of Zagreb indices, [12] and defined as follows:

$$Z1^c(G) = \sum_{uv\notin E(G)} (degu + degv),$$

$$Z2^c(G) = \sum_{uv\notin E(G)} (degu \times degv).$$

There are many studies and papers on these indices, please refer to the references [13-16]. Now, we can define these indices for single a vertex by:

$$Z1(u,G) = (degu)^2 + \sum_{uv\in E(G)} degv,$$

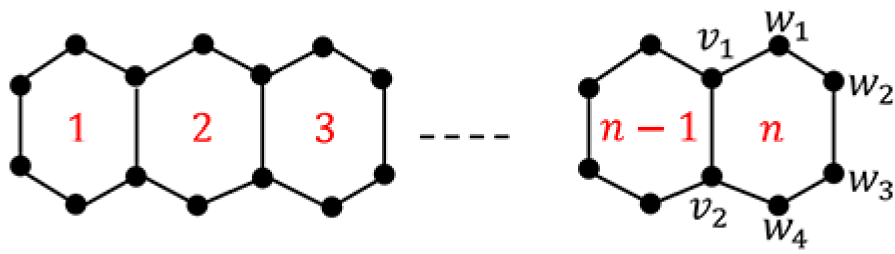


Figure 1. Chain Hexagonal Cycles (CHC_n).

$$Z2(u,G) = degu \sum_{uv \in E(G)} degv.$$

$$Z1^c(u,G) = (p - degu - 1)degu + \sum_{uv \notin E(G)} degv,$$

where p be the number of vertex set $V(G)$.

$$Z2^c(u,G) = degu \sum_{uv \notin E(G)} degv.$$

Given the importance of the properties of some chemical structures such as temperature, solubility, energy, etc., and their relationship to topological indices, such as: first Zagreb, second Zagreb, complement first Zagreb and complement second Zagreb indices. We decided to find these indices for some structures of chain of hexagonal cycles.

2 MAIN RESULTS

2.1 ZAGREB INDICES OF CHAIN HEXAGONAL CYCLES (CHC_n)

A Linear molecules are compounds having the linear geometry. That means; these linear molecules have their atomic connectivity in a straight line. All the atoms in the molecule are arranged in a perfect line. See Figure 1. In linear geometry, there are usually three atoms in the molecule – a central atom is bonded to two other atoms via covalent bonds. The two atoms in the opposite sides of this molecule are called ligands bound to the center.

Some properties of the graph CHC_n

Let n be representation the number of hexagonal cycles is, then:

(i) The order $p = p(CHC_n) = 4n + 2$ and the size $q = q(CHC_n) = 5n + 1$.

(ii) The diameter $\delta = \delta(CHC_n) = 2n + 1$.

(iii) The number of vertices have two degree is $2n+4$ and the number vertices have three degree is $2(n - 1)$.

In the following theorem, we will give the iterative formulas of the preceding evidence for the graph CHC_n.

Theorem 2.1. *For all $n \in \mathbb{Z}^+ - \{1\}$, we get:*

(i) $Z1(CHC_n) = Z1(CHC_{n-1}) + 26$.

(ii) $Z2(CHC_n) = Z2(CHC_{n-1}) + 33$.

(iii) $Z1^c(CHC_n) = Z1^c(CHC_{n-1}) + 80n - 48$.

(iv) $Z2^c(CHC_n) = Z2^c(CHC_{n-1}) + 100n - 76$.

Proof. Let w_1, w_2, w_3, w_4 be the vertices belong to $(V(CHC_n) - V(CHC_{n-1}))$ see Figure 1.

(i) From Figure 1, we can find:

$$\sum_{i=1}^{4} Z1(w_i, CHC'_{n-1}) = \sum_{i=1}^{3} [\deg(w_i) \ + \deg(w_{i+1})\ ] + [\deg(w_1) \ + \deg(v_1)]$$

$$+[\deg(w_4) \ + \deg(v_{4(n-1)+2})]$$

$$= 3(2+2) + 2(2+3) = 22,$$

where the graph CHC'_{n-1} is the graph CHC_{n-1} whose degree three for vertices of identify edge $\{v_1, v_{4(n-1)+2}\}$. Also, we add the deference between degrees ($v_1$and $v_{4(n-1)+2}$ with v_2 and $v_{4(n-1)+1}$ respectively), after adding the last hexagonal cycle and before adding the last hexagonal cycle, that is $2(3+2)+(3+3)-[2(2+2)+(2+2)] = 4$.

Hence, $Z1(CHC_n) = Z1(CHC_{n-1}) + 26$.

(ii) In the same way can get: $Z2(CHC_n) = Z2(CHC_{n-1}) + 33$.

(iii) We first find the co-index first Zagreb of vertices w_i, $i = 1, 2, 3, 4$ with vertices of $IEHC_{n-1}$. From Figure 1, we get: $Z1^c(w_i, CHC'_{n-1}) = [5(n-2)(2) + 5 + 4\ n\ (2)] = 18n - 15$, for all $i = 1, 4$. $Z1^c(w_i, CHC'_{n-1}) = [5(n-1)(2) + 4\ n\ (2)] = 18n - 10$, for all $i = 2, 3$. Now, $\sum_{i=3}^{4} [\deg(w_1) \ + \deg(w_i)] + [\deg(w_3) \ + \deg(w_4)] = 12$.

Also, we add the difference (for the vertices of identical edge) degrees after adding vertices $w_i,\ i = 1, 2, 3, 4$ and before adding them, we get:

$$2\,\{6(n-2)(2) + 5(2) + 5(n-2)(2) + 5\} - 2\,\{5(n-2)(2) + 4(2) + 4(n-2)(2) + 4\}$$

$$= 8n - 10.$$

Hence, $Z1^c(CHC_n) = Z1^c(CHC_{n-1}) + 2(18n-15) + 2(18n-10) + 12 + 8n - 10$

$$= Z1^c(CHC_{n-1}) + 80n - 48.$$

(iv) In the same way can get $Z2^c(CHC_n) = Z2^c(CHC_{n-1}) + 100n - 76$.

□

Now, we find the indices $Z1(G)$, $Z1(G)$, $Z1^c(G)$ and $Z2^c(G)$ for the identical edges for $n-$ hexagonal cycles CHC_n, $\forall\ n \in \mathbb{Z}^+ - \{1\}$.

Corollary 2.2. *For all $n \in \mathbb{Z}^+ - \{1\}$, we have:*

(i) $Z1(CHC_n) = 2(13n-1)$*, the initial value* $Z1(CHC_1) = 24$.

(ii) $Z2(CHC_n) = 3(11n-3)$*, the initial value* $Z2(CHC_1) = 24$.

(iii) $Z1^c(CHC_n) = 40n^2 - 8n + 4$*, the initial value* $Z1^c(CHC_1) = 36$.

(iv) $Z2^c(CHC_n) = 50n^2 - 26n + 12$*, the initial value* $Z2^c(CHC_1) = 36$.

Proof. (i) We use the iteration method to resolve the recurrence relation in Theorem 2.1(1). Then

$$Z1(CHC_n) = Z1(CHC_{n-1}) + 26$$
$$= Z1(CHC_{n-2}) + 26(2)$$
$$= Z1(CHC_{n-3}) + 26(3)$$
$$\vdots$$
$$= Z1(CHC_1) + 26(n-1)$$
$$= 24 + 26(n-1) = 2(13n-1).$$

(ii) In the same way can get: $Z2(CHC_n) = 3(11n-3)$.

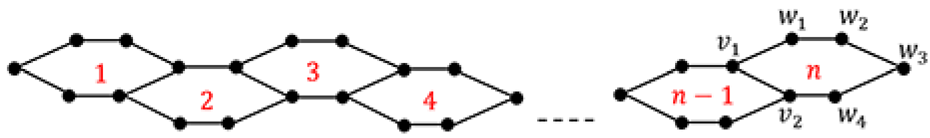


Figure 2. CHAIN ZIGZAG HEXAGONAL CYCLES $(CZHC_n)$.

(iii) Also, We use the iteration method to resolve the recurrence relation in Theorem 2.1, (3). Then

$$\begin{aligned} Z1^c(CHC_n) &= Z1^c(CHC_{n-1}) + 80n - 48 \\ &= Z1^c(CHC_{n-1}) + 80(n-1) + 32 \\ &= Z1^c(CHC_{n-2}) + 80(n-1) + 80(n-2) + 2(32) \\ &= Z1^c(CHC_{n-3}) + 80\sum_{i=1}^{3}(n-i) + 3(32) \\ &\vdots \\ &= Z1^c(CHC_1) + 80\sum_{i=1}^{n-1}(n-i) + (n-1)(32) \\ &= 36 + 40(n(n-1)) + (n-1)(32). \\ &= 40n^2 - 8n + 4. \end{aligned}$$

(iv) In the same way can get: $Z2^c(CHC_n) = 50n^2 - 26n + 12$.

□

Remark 2.3. It is possible to find many relationships between these indices and the number of vertices, or the number of edges, or the diameter by their some properties of the graph CHC_n.

2.2 ZAGRAB INDICES OF CHAIN ZIGZAG HEXAGONAL CYCLES $(CZHC_n)$

A Nonlinear molecules are compounds that have a geometry different linear geometry. That means; these molecules are not linear, and their atoms are not arranged in a straight line. The shape of these molecules depends on the hybridization of the atomic orbitals of the atoms in the molecule, see Figure 2. Some of the possible shapes are V-shaped molecules, angular, trigonal planar, tetragonal molecules, pyramidal molecules and other shapes. The bond angles of these molecules differ from each other according to the shape.

It is clear that $CZHC_n$ has the same order, size, diameter and the number of vertices which have degree two and three as the CHC_n, $n \in \mathbb{Z}^+$.

In the following theorem, we will give the iterative formulas general of Zagreb indices for the graph $CZHC_n$.

Theorem 2.4.

$$1. Z1(CZHC_n) = Z1(CZHC_{n-1}) + 26, n \in \mathbb{Z}^+ - \{1\}.$$

$$2. Z2(CZHC_n) = Z2(CZHC_{n-1}) + 34, n \in \mathbb{Z}^+ - \{1, 2\}.$$

$$3. Z1^c(CZHC_n) = Z1^c(CZHC_{n-1}) + 80n - 48, n \in \mathbb{Z}^+ - \{1\}.$$

$$4. Z2^c(CZHC_n) = Z2^c(CZHC_{n-1}) + 100n - 77, n \in \mathbb{Z}^+ - \{1, 2\}.$$

Proof. We will only prove the second and fourth, because one and three are mentioned in the Theorem 2.1. Let w_1, w_2, w_3, w_4 be the vertices belong to $(V(CZHC_n) - V(CZHC_{n-1}))$ see Figure 2.

2. From Figure 2, we can find:

$$\sum_{i=1}^{4} Z2(w_i, CZHC'_{n-1}) = \sum_{i=1}^{3} [\deg(w_i) \times \deg(w_{i+1})] + [\deg(w_1) \times \deg(v_1)]$$

$$+[\deg(w_4) \times \deg(v_{4(n-1)+2})] = 3(2\times 2) + 2(2\times 3) = 24,$$

where the graph $CZHC'_{n-1}$ is the graph $CZHC_{n-1}$ whose degree three for vertices of identify edge $\{v_1, v_{4(n-1)+2}\}$. Also, we add the difference between degrees ($v_1$and $v_{4(n-1)+2}$ with v_2 and $v_{4(n-1)+1}$ respectively), after adding the last hexagonal cycle and before adding the last hexagonal cycle, that is $(3\times 2) + 2(3\times 3) - [2(2\times 2) + (3\times 2)] = 10$. Hence, $Z2(CZHC_n) = Z2(CZHC_{n-1}) + 34$.

4. We first find the co-index first Zagreb of vertices w_i, $i = 1,2,3,4$ with vertices of $CZHC_{n-1}$. From Figure 2, we get:

$$Z2^c(w_i, CZHC'_{n-1}) = [6(n-2)(2) + 6 + 4\,n\,(2)] = 20n - 18, \text{ for all } i = 1,4.$$

$$Z2^c(w_i, CZHC'_{n-1}) = [6(n-1)(2) + 4\,n\,(2)] = 20n - 12, \text{ for all } i = 2,3.$$

Now, $\sum_{i=3}^{4} [\deg(w_1) \times \deg(w_i)] + [\deg(w_2) \times \deg(w_4)] = 12$.

Also, we add the difference degrees for vertices $v_1$and $v_{4(n-1)+2}$ (identical vertices) after adding the last hexagonal cycle and before adding the last hexagonal cycle, we get:

$$\{9(n-2)(2) + 6(n-1)(2) + 6\} + \{9(n-3)(2) + 9 + 6n(2)\}$$

$$-\{6(n-2)(2) + 4(n-1)(2) + 4\} - \{6(n-3)(2) + 6 + 4n(2)\} = 20n - 29.$$

Hence, $Z2^c(CZHC_n) = Z2^c(CZHC_{n-1}) + 2(20n-18) + 2(20n-12) + 12 + 20n - 29$

$$= Z2^c(CZHC_{n-1}) + 100n - 77.$$

□

Now, we find the indices $Z1(G)$, $Z2(G)$, $Z1^c(G)$ and $Z2^c(G)$ for the zigzag identical edges for $n-$ hexagonal cycles $CZHC_n$, $\forall\, n \in \mathbb{Z}^+ - \{1\}$.

Corollary 2.5. *For all $n \in \mathbb{Z}^+ - \{1\}$, we have:*

(i) $Z1(CZHC_n) = 2(13n-1)$, *the initial value* $Z1(CZHC_1) = 24$.

(ii) $Z2(CZHC_n) = 34n - 11$, *the initial value* $Z2(CZHC_2) = 57$.

(iii) $Z1^c(CZHC_n) = 40n^2 - 8n + 4$, *the initial value* $Z1^c(CZHC_1) = 36$.

(iv) $Z2^c(CZHC_n) = 50n^2 - 27n + 14$, *the initial value* $Z2^c(CZHC_2) = 160$.

Proof. ii. We use the iteration method to resolve the recurrence relation in Theorem 2.4,(2). Then

$$\begin{aligned} Z2(CZHC_n) &= Z2(CZHC_{n-1}) + 34, n \in \mathbb{Z}^+ - \{1,2\}. \\ &= Z2(CZHC_{n-2}) + 34(2) \\ &= Z2(CZHC_{n-3}) + 34(3) \\ &\vdots \\ &= Z2(CZHC_2) + 34(n-2) \\ &= 57 + 34(n-2) = 34n - 11. \end{aligned}$$

Hence, $Z2(CZHC_n) = 34n - 11$, for all $n \in \mathbb{Z}^+$.

iv. Also, we use the iteration method to resolve the recurrence relation in Theorem 2.4,(4). Then

$$\begin{aligned}
Z2^c(CZHC_n) &= Z2^c(CZHC_{n-1}) + 100n - 77\\
&= Z2^c(CZHC_{n-2}) + 100n + 100(n-1) - 2(77)\\
&= Z2^c(CZHC_{n-3}) + 100\sum_{i=0}^{2}(n-i) - 3(77)\\
&\ \vdots\\
&= Z2^c(CZHC_2) + 100\sum_{i=0}^{n-3}(n-i) - (n-2)(77)\\
&= 36 + 40(n(n-1)) + (n-1)(32).\\
&= 50n^2 - 27n + 14.
\end{aligned}$$

□

Remark 2.6. It is possible to find many relationships between these indices and the number of vertices, or the number of edges, or the diameter by their some properties of the graph $CZHC_n$.

3 SOME EXAMPLES OF CHEMICAL STRUCTURES

All materials have different physical and chemical properties; also have physical or chemical changes. Physical properties, such as hardness and boiling point, and physical changes, such as melting or freezing, do not include a change in the composition of matter. Chemical properties, such flammability and acidity, and chemical changes, such as rusting, involve production of matter that differs from that present beforehand. In tables 1 and 2 all chemical structures and their physical properties and changes in linear and angular acene were illustrated.

A topological graph index, and also refer to a molecular descriptor, is a mathematical formula that can be applied to any graph and using it to models some molecular structure as well as to analysis mathematical values and more looking for some physicochemical properties of a molecule. Therefore, it is an efficient method to avoid expensive and time-consuming laboratory experiments. Therefore, our goal in this paper was to find some topological indices that shows the relationship between chemical properties and mathematical formulas through algebraic formulas of the second or third degree.

Example 3.1. When considering organic compounds having the linear geometry, there is a Carbon atom at the center of the molecule, and the ligands bind with the carbon atom via double or triple bonds. For example, Benzene is an organic chemical compound with the molecular formula C_6H_6. Also we take the structures, Naphthalene, Anthracene, Tetracene, Pentacene, Hexacene, Heptacene, Octacene and Nonacene. Because these structures contain only carbon and hydrogen atoms, therefore can be classified as a hydrocarbon. In addition to the previous, there are linear inorganic compounds as well; for example, carbon dioxide, hydrogen cyanide, and so on, [17,18].

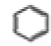
Table 1 illustrated some chemical properties for each compound starts with the compound that consist of single hexagonal ring represented by Benzene and ending with the compound that consist of nine hexagonal ring represented by Nonacene.

Now, we will find the relationship between ZAGREB Indices and some chemical properties like: Boiling point and Melting point, by using Excel and making a test for all types of mathematical functions (linear, quadratic, cubic and special functions), and notice that which of the formula is the best compared with the real values of chemical properties.

From the Figure 3, we notice that the best topological indices are $Z1(C_{4n+2}H_{2n+4})$ and $Z2(C_{4n+2}H_{2n+4})$, as the first Zagreb is more accurate and less error.

From the Figure 4, $Z1(C_{4n+2}H_{2n+4})$ and $Z2(C_{4n+2}H_{2n+4})$ are the best, and first Zagreb is more accurate and less error.

Table 1. Some Properties of $C_{4n+2}H_{2n+4}$, $n = 1, 2, \ldots, 9$, [19].

	Compound name	Molecular Weight	Melting Point (°C):	Boiling Point (°C):	Density (g/cm3 at 25°C)	Molar Volume (cm3/mol): (25°C)	Compound shape
1	Benzene. C6H6	78.112	5.49	78.8±7.0	0.9 ± 0.1	89.4±3.0	
2	Naphthalene C10H8	128.171	77-82	221.5±7.0	1.0 ± 0.1	123.5±3.0	
3	Anthracene C14H10	178.229	78.09	337.4±9.0	1.1 ± 0.1	157.7±3.0	
4	Tetracene C18H12	228.288	135.96	436.7±12.0	1.2 ± 0.1	191.8±3.0	
5	Pentacene C22H14	278.346	180.52	524.7±17.0	1.2 ± 0.1	225.9±3.0	
6	Hexacene C26H16	328.405	231.70	604.1±22.0	1.3 ± 0.1	260.0±3.0	
7	Heptacene C30H18	378.474	264.86	677.0±22.0	1.3 ± 0.1	294.1±3.0	
8	Octacene C34H20	428.499	297.98	744.7±27.0	1.3 ± 0.1	328.2±3.0	
9	Nonacene C38H22	478.594	331.10	753.68	1.3 ± 0.1	362.4±3.0	

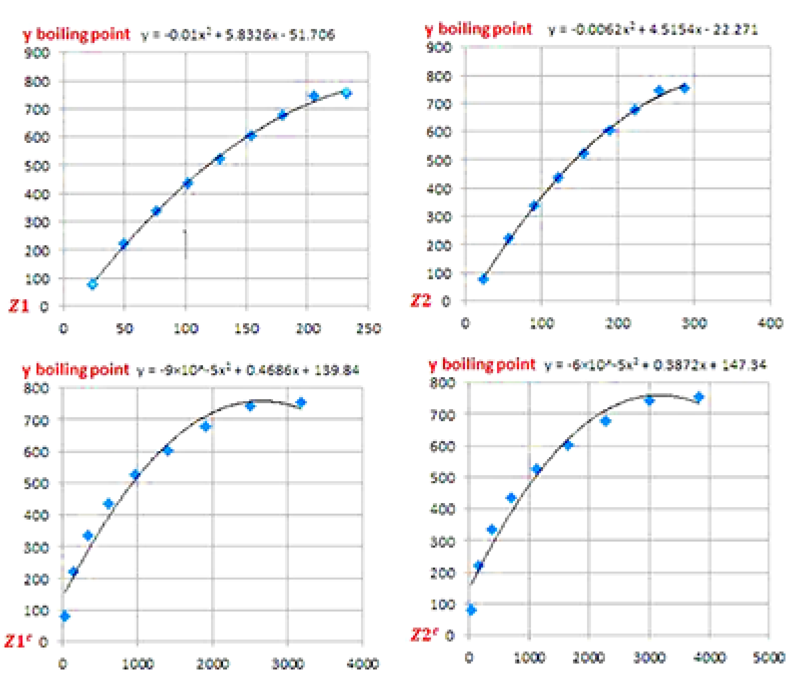


Figure 3. Zagreb indices with boiling point of $C_{4n+2}H_{2n+4}$, $n = 1, 2, \ldots, 9$.

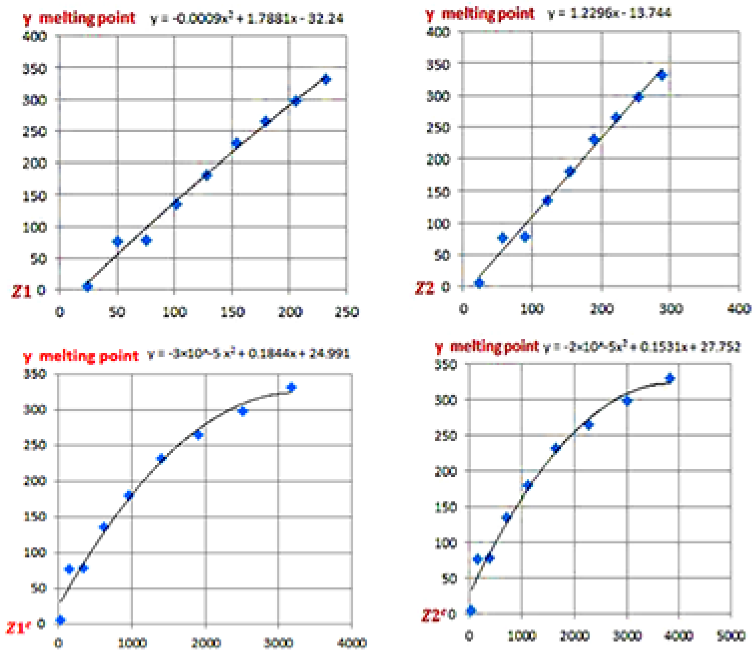
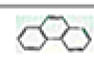
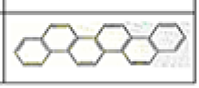


Figure 4. Zagreb indices with melting point of $C_{4n+2}H_{2n+4}$, $n = 1, 2, \ldots, 9$.

Table 2. Some Properties of $C_{4n+2}H_{2n+4}$, $n = 1, 2, 3, 4, 5, 6$, [19].

	Compound name	Molecular Weight	Melting Point (°C):	Boiling Point (°C):	Density (g/cm3) at 20°C)	Molar Vol. (cm3/mol):(20°C)	Compound shape
1	Benzene. C6H6	78.112	5.49	78.8±7.0	0.9 ± 0.1	89.4±3.0	
2	Naphthalene C10H8	128.171	80.26	218.0	1.0253 1.0±0.1	123.5±3.0	
3	Phenanthrene C14H10	178.229	99.24	340.0	1.174 1.1±0.1	157.7±3.0	
4	Chrysene C18H12	228.288	255.2	448.0	1.274 1.2±0.1	191.8±3.0	
5	Picene C22H14	278.347	368.0	519.0	1.2±0.1	225.9±3.0	
6	benzo[e]picene C26H16	328.405	395.70	604.1±22.0	1.3±0.1	260.0±3.0	

Example 3.2. When considering complex molecules such as polymers, they also can be linear or nonlinear. Most of the nonlinear polymers are branched or cross-linked polymers. Branched polymers have side groups or pendant groups attached to a straight line of atoms. Cross-linked polymers have cross-links between straight lines of polymer chains that have form of network structures. For this case, we take these chemical structures: Phenanthrene, Chrysene, Picene, Benzo[e]picene, [20].

Table 2 illustrated some chemical properties for each compound starts with the compound that consist of single hexagonal ring represented by Benzene and ending with the compound that consist of six hexagonal ring represented by Benzo[e]picene.

Also, as the same as the previous method, we will find the relationship between ZAGREB Indices and some chemical properties like.

From the Figure 5, we notice that the best topological indices are $Z1(C_{4n+2}H_{2n+4})$ and $Z2^c(C_{4n+2}H_{2n+4})$, as the first Zagreb is more accurate and less error.

From the Figure 6, we notice that the best topological indices is $Z1(C_{4n+2}H_{2n+4})$ which is more accurate and less error.

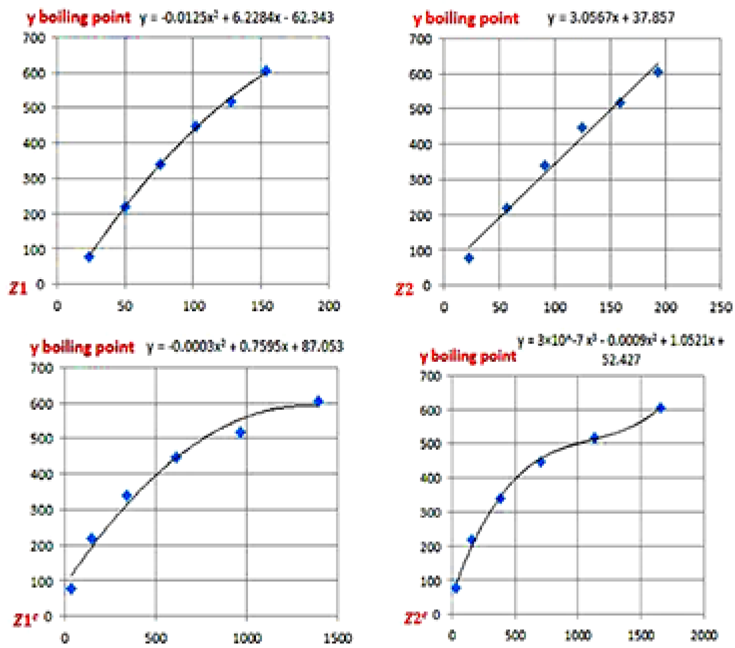


Figure 5. Zagreb indices with boiling point of $C_{4n+2}H_{2n+4}$, $n = 1, 2, \ldots, 6$.

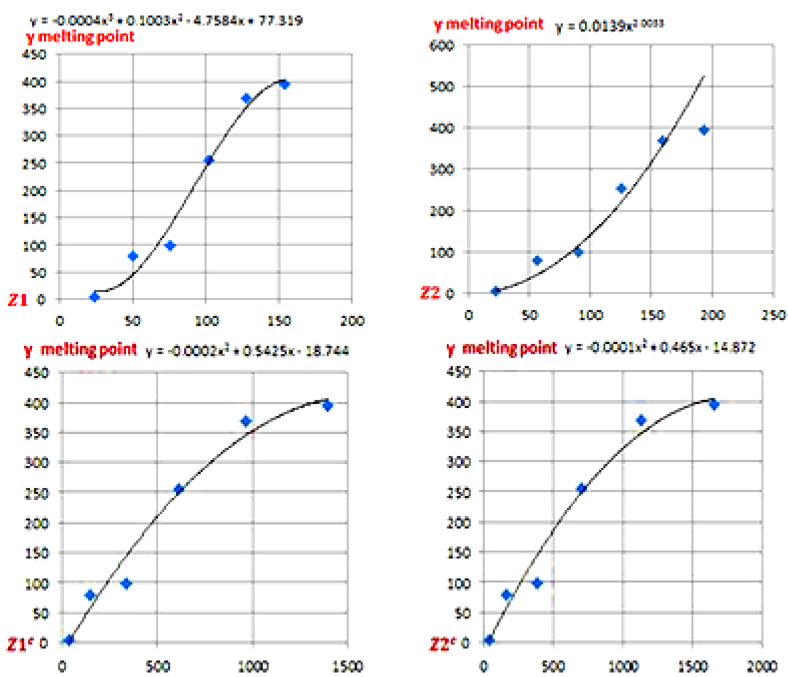


Figure 6. Zagreb indices with melting point of $C_{4n+2}H_{2n+4}$, $n = 1, 2, \ldots, 6$.

4 Conclusion

After studying and investigating, we found it is not possible to find a relationship between topological indices (Zagreb indices) and the properties (Molar volume and Density) by finding many formulas between them because there were a very big error.

By comparing the values of boiling point and melting point for structures in Examples 3.1 and 3.2 with each indices $Z1$, $Z2$, $Z2^c$ via curve fitting using (linear, quadratic, cubic and special functions) for each case, we conclude that the first and the second graphs are better than others because the mean square error is very small.

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