DEGREE-BASED TOPOLOGICAL INDICES OF $TUC_4C_8(S)$ NANOTUBES

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$TUC_4C_8(S)$ nanotubes belong to important and extensively studied compounds in materials science. Topological indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties. These nanotubes can be represented by graphs which consist of vertices and edges. Several researchers studied one or a few chosen topological indices for $TUC_4C_8(S)$ nanotubes. We obtained a general formula presented in our first theorem. The importance of our formula is that it is not necessary to do a complicated investigation in order to find one particular degree-based index for $TUC_4C_8(S)$ nanotubes. It suffices to take the definition of a particular index and use it our formula. We used our formula to obtain the second theorem containing the most well-known indices for $TUC_4C_8(S)$ nanotubes.

Keywords: degree-based index, topological index, nanotube.

1. Introduction

Molecular descriptors called topological indices are graph invariants that play a significant role in chemistry, materials science, pharmaceutical sciences and engineering, since they can be correlated with a large number of physico-chemical properties of molecules. Topological indices are used in the process of correlating the chemical structures with various characteristics such as boiling points and molar heats of formation. Graph theory is used to characterize these chemical structures.

Topological indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties. These indices are a convenient method of translating chemical constitution into numerical values which are used for correlations with physical properties.

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. The vertices and the edges of G are used to represent the atoms and the bonds of chemical structures. The number of edges incident with a vertex $x \in V(G)$ is the degree of x, denoted by d_x.

Carbon nanotubes are the stiffest and strongest materials yet discovered in terms of tensile strength and elastic modulus. They have outstanding thermal conductivity, useful absorption, mechanical and electrical properties.

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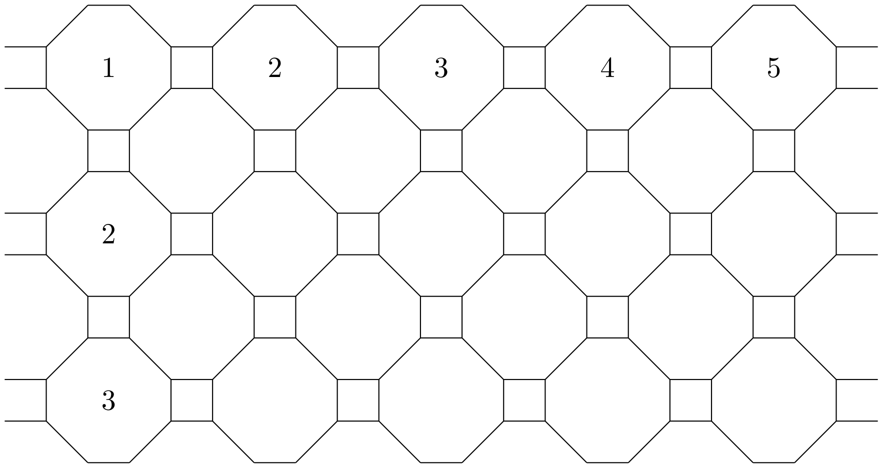

Fig. 1. $TUC_4C_8(S)$ nanotube for $p = 5$ and $q = 3$.

These nanotubes are semiconducting or metalic along the tubular axis. Carbon nanotubes can be applied as additives to various structural materials. For more details, see [14].

$TUC_4C_8(S)$ nanotubes belong to extensively studied compounds in materials science. The geometric-arithmetic index of $TUC_4C_8(S)$ nanotubes was presented in [7] and indices related to the geometric-arithmetic index were studied also in [10] and [13]. The hyper-Zagreb index of nanotubes with different number of edges was considered in [4]. The Cluj index of $TUC_4C_8(S)$ nanotubes was investigated in [8], the PI index in [3], the edge-PI index in [9] and some connectivity indices were studied in [5]. $TUC_4C_8(S)$ nanotubes were considered also in [15] and some other nanotubes were considered in [1], [2], [6], [11] and [16].

We present a general formula and use it to obtain any index based on degrees for $TUC_4C_8(S)$ nanotubes. The formula can be used to obtain also topological indices which might be introduced in the future.

We investigate an invariant $I(G)$ which is defined as follows:

$$I(G) = \sum_{xy \in E(G)} g(d_x, d_y),$$

where $g(d_x, d_y)$ is a real function of d_x and d_y, and $g(d_x, d_y) = g(d_y, d_x)$.

If $g(d_x, d_y) = (d_x d_y)^a$ where $a \in \mathbb{R}$, $a \neq 0$, $I(G)$ is the general Randić index of G,

$$R_a(G) = (d_x d_y)^a. \tag{1}$$

$R_a(G)$ is the Randić index for $a = -\frac{1}{2}$, the second Zagreb index for $a = 1$ and the second modified Zagreb index for $a = -1$.

If $g(d_x, d_y) = (d_x + d_y)^a$, we obtain the general sum-connectivity index of G,

$$X_a(G) = (d_x + d_y)^a. \tag{2}$$

Note that $X_a(G)$ is the sum-connectivity index for $a = -\frac{1}{2}$, the first Zagreb index for $a = 1$ and the hyper-Zagreb index for $a = 2$.

If $g(d_x, d_y) = d_x^a d_y^b + d_y^a d_x^b$, we obtain the generalized Zagreb index

$$GZ(G) = d_x^a d_y^b + d_y^a d_x^b. \tag{3}$$

If $g(d_x, d_y) = \frac{2}{d_x+d_y}$, we get the harmonic index

$$H(G) = \frac{2}{d_x + d_y}. \tag{4}$$

If $g(d_x, d_y) = \frac{\sqrt{d_x d_y}}{\frac{1}{2}(d_x+d_y)}$, we obtain the geometric-arithmetic index

$$GA(G) = \frac{\sqrt{d_x d_y}}{\frac{1}{2}(d_x + d_y)}. \tag{5}$$

If $g(d_x, d_y) = \frac{d_x^2+d_y^2}{d_x d_y}$, we get the symmetric division deg index

$$SDD(G) = \frac{d_x^2 + d_y^2}{d_x d_y}. \tag{6}$$

If $g(d_x, d_y) = \sqrt{\frac{d_x+d_y-2}{d_x d_y}}$, we obtain the atom-bond connectivity index

$$ABC(G) = \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}. \tag{7}$$

If $g(d_x, d_y) = \left(\frac{d_x d_y}{d_x+d_y-2}\right)^3$, we get the augmented Zagreb index

$$AZI(G) = \left(\frac{d_x d_y}{d_x + d_y - 2}\right)^3. \tag{8}$$

If $g(d_x, d_y) = \frac{1}{\max\{d_x,d_y\}}$, we obtain the variation of the Randić index

$$R'(G) = \frac{1}{\max\{d_x, d_y\}}. \tag{9}$$

If $g(d_x, d_y) = \frac{d_x+d_y}{d_x d_y}$, then $I(G)$ is the first redefined Zagreb index

$$ReZG_1(G) = \frac{d_x + d_y}{d_x d_y}. \tag{10}$$

If $g(d_x, d_y) = \frac{d_x d_y}{d_x+d_y}$, we get the second redefined Zagreb index

$$ReZG_2(G) = \frac{d_x d_y}{d_x + d_y}. \tag{11}$$

If $g(d_x, d_y) = d_x d_y(d_x + d_y)$, then $I(G)$ is the third redefined Zagreb index

$$ReZG_3(G) = d_x d_y(d_x + d_y). \tag{12}$$

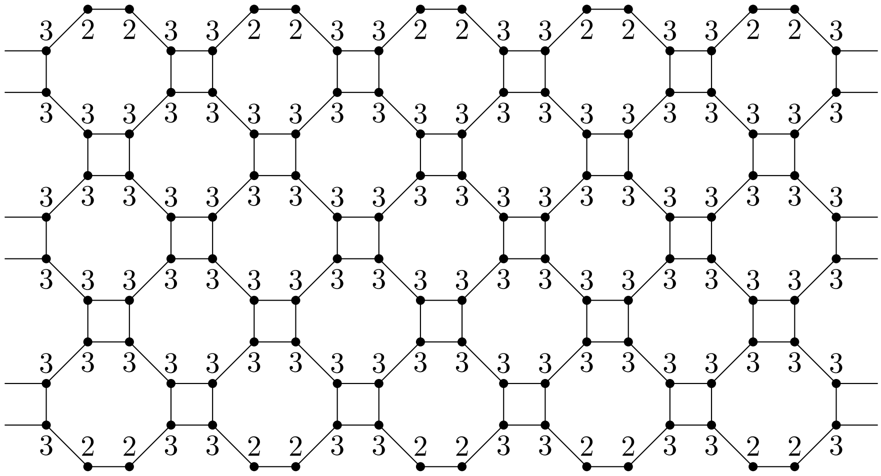

Fig. 2. $TUC_4C_8(S)$ nanotube with degrees assigned to the vertices for $p = 5$ and $q = 3$.

2. **Results**

The two-dimensional lattice of the $TUC_4C_8(S)$ nanotube for $p = 5$ and $q = 3$ is given in Fig. 1. Note that p is the number of octagons in each row and q is the number of octagons in each column, where p and q are positive integers.

Let us present a general formula and use it to obtain indices based on degrees for $TUC_4C_8(S)$ nanotubes.

Theorem 2.1. *Let G be the $TUC_4C_8(S)$ nanotube. Then*

$$I(G) = \sum_{xy \in E(G)} g(d_x, d_y) = [(6q-4) \cdot g(3,3) + 2 \cdot g(3,2) + g(2,2)]2p. \quad (13)$$

Proof. Since every octagon contains 8 vertices, the number of vertices in this nanotube is equal to $8pq$ (see Fig. 2). Every vertex has degree 2 or 3. We have $4p$ vertices of degree 2 and the other vertices have degree 3. Similarly, every octagon contains 8 edges. There are $2pq$ other horizontal edges and $2p(q-1)$ other vertical edges (see Fig. 2), thus the number of edges in G is $8pq + 2pq + 2p(q-1) = 2p(6q-1)$. Let

$$E_{i,j} = \{xy \in E(G) \mid d_x = i,\ d_y = j\}.$$

This means that the set $E_{i,j}$ contains the edges incident with one vertex of degree i and the other vertex of degree j. We have $E(G) = E_{2,2} \cup E_{3,2} \cup E_{3,3}$. Clearly, $|E_{2,2}| = 2p$, because there are $2p$ edges with both end-vertices having degree 2. Since each of the $4p$ vertices having degree two is adjacent to one vertex having degree three, we get $|E_{3,2}| = 4p$. Thus $|E_{3,3}| = |E(G)| - |E_{2,2}| -$

$|E_{3,2}| = 2p(6q-4)$ and

$$\begin{aligned} I(G) &= \sum_{xy\in E(G)} g(d_x,d_y) = \sum_{xy\in E_{3,3}} g(3,3) + \sum_{xy\in E_{3,2}} g(3,2) + \sum_{xy\in E_{2,2}} g(2,2) \\ &= 2p(6q-4)\cdot g(3,3) + 4p\cdot g(3,2) + 2p\cdot g(2,2) \\ &= [(6q-4)\cdot g(3,3) + 2\cdot g(3,2) + g(2,2)]2p. \end{aligned}$$

□

Now we obtain values of many indices based on degrees for $TUC_4C_8(S)$ nanotubes.

Theorem 2.2. *Let G be the $TUC_4C_8(S)$ nanotube. Then the general Randić index of G,*

$$R_a(G) = [(6q-4)\cdot 9^a + 2\cdot 6^a + 4^a]2p,$$

the Randić index

$$R_{-\frac{1}{2}}(G) = \left(4q + \frac{2\sqrt{6}-5}{3}\right)p,$$

the second Zagreb index

$$R_1(G) = (27q-10)4p,$$

the second modified Zagreb index

$$R_{-1}(G) = \left(\frac{4q}{3} + \frac{5}{18}\right)p,$$

the general sum-connectivity index

$$X_a(G) = [(6q-4)\cdot 6^a + 2\cdot 5^a + 4^a]2p,$$

the sum-connectivity index

$$X_{-\frac{1}{2}}(G) = \left(2\sqrt{6}q + \frac{12\sqrt{5}-20\sqrt{6}}{15} + 1\right)p,$$

the first Zagreb index

$$X_1(G) = (18q-5)4p,$$

the hyper-Zagreb index

$$X_2(G) = (108q-39)4p,$$

the generalized Zagreb index

$$GZ(G) = (3^{a+b+1}2q - 3^{a+b}4 + 3^a2^b + 2^a3^b + 2^{a+b})4p,$$

the harmonic index

$$H(G) = \left(4q - \frac{1}{15}\right)p,$$

the geometric-arithmetic index

$$GA(G) = \left(12q + \frac{8\sqrt{6} - 30}{5}\right) p,$$

the symmetric division deg index

$$SDD(G) = \left(24q - \frac{10}{3}\right) p,$$

the atom-bond connectivity index

$$ABC(G) = \left(8q + \frac{9\sqrt{2} - 16}{3}\right) p,$$

the augmented Zagreb index

$$AZI(G) = \left(\frac{2187q}{16} - \frac{345}{8}\right) p,$$

the variation of the Randić index

$$R'(G) = \left(4q - \frac{1}{3}\right) p,$$

the first redefined Zagreb index

$$ReZG_1(G) = 8qp,$$

the second redefined Zagreb index

$$ReZG_2(G) = \left(18q - \frac{26}{5}\right) p$$

and the third redefined Zagreb index

$$ReZG_3(G) = (81q - 35)8p.$$

Proof. If $R_a(G)$ is the general Randić index defined in (1), we obtain $g(d_x, d_y) = (d_x d_y)^a$. Since $g(3,3) = 9^a$, $g(3,2) = 6^a$ and $g(2,2) = 4^a$, by (13),

$$R_a(G) = [(6q-4)9^a + 2 \cdot 6^a + 4^a]2p.$$

For $a = -\frac{1}{2}$ the Randić index is

$$R_{-\frac{1}{2}}(G) = \left(\frac{6q-4}{3} + \frac{2}{\sqrt{6}} + \frac{1}{2}\right) 2p = \left(4q + \frac{2\sqrt{6} - 5}{3}\right) p.$$

For $a = 1$ we get the second Zagreb index

$$R_1(G) = [(6q-4)9 + 2 \cdot 6 + 4]2p = (27q - 10)4p.$$

For $a = -1$ the second modified Zagreb index is

$$R_{-1}(G) = \left(\frac{6q-4}{9} + \frac{2}{6} + \frac{1}{4}\right) 2p = \left(\frac{4q}{3} + \frac{5}{18}\right) p.$$

For $X_a(G)$ that is the general sum-connectivity index defined in (2), $g(d_x, d_y) = (d_x + d_y)^a$, thus $g(3, 3) = 6^a$, $g(3, 2) = 5^a$ and $g(2, 2) = 4^a$. Then by (13),

$$X_a(G) = [(6q - 4)6^a + 2 \cdot 5^a + 4^a]2p.$$

For $a = -\frac{1}{2}$ the sum-connectivity index is

$$X_{-\frac{1}{2}}(G) = \left(\frac{6q-4}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2}\right) 2p = \left(2\sqrt{6}q + \frac{12\sqrt{5} - 20\sqrt{6}}{15} + 1\right) p.$$

For $a = 1$ the first Zagreb index is

$$X_1(G) = [(6q - 4)6 + 2 \cdot 5 + 4]2p = (18q - 5)4p.$$

For $a = 2$ the hyper-Zagreb index is

$$X_2(G) = [(6q - 4)6^2 + 2 \cdot 5^2 + 4^2]2p = (108q - 39)4p.$$

For $GZ(G)$ that is the generalized Zagreb index presented in (3), we obtain $g(d_x, d_y) = d_x^a d_y^b + d_y^a d_x^b$. Since $g(3, 3) = 3^a 3^b 2 = 3^{a+b}2$, $g(3, 2) = 3^a 2^b + 2^a 3^b$ and $g(2, 2) = 2^a 2^b 2 = 2^{a+b}2$, by (13),

$$\begin{aligned} GZ(G) &= [(6q - 4)3^{a+b}2 + 2(3^a 2^b + 2^a 3^b) + 2^{a+b}2]2p \\ &= (3^{a+b+1}2q - 3^{a+b}4 + 3^a 2^b + 2^a 3^b + 2^{a+b})4p. \end{aligned}$$

For $H(G)$ which is the harmonic index defined in (4), we obtain $g(d_x, d_y) = \frac{2}{d_x+d_y}$, thus $g(3, 3) = \frac{1}{3}$, $g(3, 2) = \frac{2}{5}$ and $g(2, 2) = \frac{1}{2}$. Therefore, by (13),

$$H(G) = \left[(6q - 4)\frac{1}{3} + 2 \cdot \frac{2}{5} + \frac{1}{2}\right] 2p = \left(4q - \frac{1}{15}\right) p.$$

For the geometric-arithmetic index $GA(G)$ given in (5), we get $g(d_x, d_y) = \frac{\sqrt{d_x d_y}}{\frac{1}{2}(d_x+d_y)}$. Since $g(3, 3) = 1$, $g(3, 2) = \frac{2\sqrt{6}}{5}$ and $g(2, 2) = 1$, we obtain

$$GA(G) = \left[(6q - 4) + 2 \cdot \frac{2\sqrt{6}}{5} + 1\right] 2p = \left(12q + \frac{8\sqrt{6} - 30}{5}\right) p.$$

For $SDD(G)$ that is the symmetric division deg index introduced in (6), we obtain $g(d_x, d_y) = \frac{d_x^2+d_y^2}{d_x d_y}$. Then $g(3, 3) = 2$, $g(3, 2) = \frac{13}{6}$ and $g(2, 2) = 2$, so by (13),

$$SDD(G) = \left[(6q - 4)2 + 2 \cdot \frac{13}{6} + 2\right] 2p = \left(24q - \frac{10}{3}\right) p.$$

For $ABC(G)$ which is the atom-bond connectivity index defined in (7), we obtain $g(d_x, d_y) = \sqrt{\frac{d_x+d_y-2}{d_x d_y}}$, so $g(3, 3) = \frac{2}{3}$, $g(3, 2) = \frac{1}{\sqrt{2}}$ and $g(2, 2) = \frac{1}{\sqrt{2}}$. Therefore by (13),

$$ABC(G) = \left[(6q - 4)\frac{2}{3} + 2 \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}}\right] 2p = \left(8q + \frac{9\sqrt{2} - 16}{3}\right) p.$$

For $AZI(G)$ that is the augmented Zagreb index given in (8), we obtain $g(d_x, d_y) = (\frac{d_x d_y}{d_x + d_y - 2})^3$. Then $g(3,3) = \frac{729}{64}$, $g(3,2) = 8$ and $g(2,2) = 8$. Thus

$$AZI(G) = \left[(6q-4)\,\frac{729}{64} + 2\cdot 8 + 8\right] 2p = \left(\frac{2187q}{16} - \frac{345}{8}\right) p.$$

For $R'(G)$ which is the variation of the Randić index defined in (9), we get $g(d_x, d_y) = \frac{1}{\max\{d_x, d_y\}}$, so $g(3,3) = g(3,2) = \frac{1}{3}$ and $g(2,2) = \frac{1}{2}$. Therefore by (13),

$$R'(G) = \left(\frac{6q-4}{3} + \frac{2}{3} + \frac{1}{2}\right) 2p = \left(4q - \frac{1}{3}\right) p.$$

For the first redefined Zagreb index $ReZG_1(G)$ introduced in (10), we obtain $g(d_x, d_y) = \frac{d_x + d_y}{d_x d_y}$, thus $g(3,3) = \frac{2}{3}$, $g(3,2) = \frac{5}{6}$ and $g(2,2) = 1$. So

$$ReZG_1(G) = \left[(6q-4)\frac{2}{3} + 2\cdot\frac{5}{6} + 1\right] 2p = 8qp.$$

For the second redefined Zagreb index $ReZG_2(G)$ given in (11), we get $g(d_x, d_y) = \frac{d_x d_y}{d_x + d_y}$, thus $g(3,3) = \frac{3}{2}$, $g(3,2) = \frac{6}{5}$ and $g(2,2) = 1$. Therefore by (13),

$$ReZG_2(G) = \left[(6q-4)\frac{3}{2} + 2\cdot\frac{6}{5} + 1\right] 2p = \left(18q - \frac{26}{5}\right) p.$$

For the third redefined Zagreb index $ReZG_3(G)$ defined in (12), we obtain $g(d_x, d_y) = (d_x + d_y) d_x d_y$, thus $g(3,3) = 54$, $g(3,2) = 30$ and $g(2,2) = 16$. Hence by (13),

$$ReZG_3(G) = [(6q-4)54 + 2\cdot 30 + 16]2p = (81q - 35)8p.$$

□

3. **Conclusion**

Topological indices of nanotubes are numerical descriptors that are derived from graphs of chemical compounds. It was described for example in [12] that topological indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties. These nanotubes can be represented by graphs which consist of vertices and edges.

Several researchers studied one or a few chosen topological indices for $TUC_4C_8(S)$ nanotubes (see [3], [4], [5], [8], [7], [9], [10] and [13]). Our goal was to get a formula which can be used to obtain any degree-based index for those nanotubes. We succeeded and obtained general formula (13) presented in Theorem 2.1. The importance of formula (13) is that it is not necessary to do a complicated investigation in order to find one particular degree-based index for $TUC_4C_8(S)$ nanotubes. It suffices to take the definition of a particular index and use it in formula (13).

For example, the hyper-Zagreb index is defined as

$$\sum_{xy\in E(G)} g(d_x, d_y) = \sum_{xy\in E(G)} (d_x + d_y)^2,$$

see Section 1. It is easy to compute $g(3,3)$, $g(3,2)$ and $g(2,2)$. We get $g(3,3) = (3+3)^2 = 36$, $g(3,2) = (3+2)^2 = 25$ and $g(2,2) = (2+2)^2 = 14$. Then we use formula (13) to compute the hyper-Zagreb index. We get

$$[(6q-4)\cdot g(3,3)+2\cdot g(3,2)+g(2,2)]2p = [(6q-4)36+2\cdot 25+16]2p = (108q-39)4p,$$

We used formula (13) to obtain Theorem 2.2 containing the most well-known indices for $TUC_4C_8(S)$ nanotubes. However, even those indices which are not presented in Theorem 2.2 or indices which might be introduced in the future can be easily computed using formula (13).

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