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GENERAL FORMULA FOR DEGREE-BASED TOPOLOGICAL INDICES OF TITANIA NANOTUBES

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Molecular descriptors known as topological indices are graphical invariants which are used in chemistry, pharmaceutical sciences, materials science and engineering, because we can correlate these indices with a big number of chemical and physical properties of molecules. For titania nanotubes, we present the values of the most famous indices including Randić indices which are named after the chemist Milan Randić. Those indices are used to correlate the chemical structures and characteristics including boiling points and molar heats of formation. We focus on titania nanotubes, because they belong to the most studied compounds in materials science.

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

1. Introduction

Because of the exceptional properties of titania nanotubes, these nanotubes are used for instance in photocatalysis, biomedical devices and dye-sensitized solar cells. Bulk TiO_2 is a corrosion-resistant and non-toxic material friendly to the environment.

The chemical structure of a molecule is represented by molecular descriptors. Currently, there is enormously large research in the area of the computation of these topological indices for various chemical frameworks. We use graph theory to investigate the chemical structures.

Let G be a simple connected graph G with vertex set $V(G)$ and edge set $E(G)$. The number of vertices adjacent to a vertex $x \in V(G)$ is the degree d_x of x. The atoms and bonds of chemical structures are represented by the vertices and edges of graphs.

Malik and Imran [10] presented the Zagreb indices of titania nanotubes $TiO_2[m,n]$, Gao et al. [5] obtained the redefined Zagreb indices for $TiO_2[m,n]$ nanotubes, Gao, Farahani and Imran [4] presented the sum-connectivity index, the Randić index and the modified Randić index for these nanotubes. The Randić index and the redefined second Zagreb index were corrected in [13]. Javaid et al. [8] obtained the generalized Zagreb index of $TiO_2[m,n]$ nanotubes.

Different titania networks containing also edges with both end-vertices of degree 2 were investigated in [3] and [11]. Titania networks containing vertices

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of degree 1 were considered in [14]. Indices for nanotubes and other chemical graphs were studied also in [1], [2], [7] and [12].

We obtain a general formula that can be applied to obtain any degree-based index (defined by the sum for the edges) for titania nanotubes. Then we present the values of the most famous indices based on degrees for titania nanotubes. We investigate an invariant

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

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

- If $f(d_x, d_y) = (d_x d_y)^\alpha$ for real numbers $\alpha \neq 0$, we obtain the general Randić index $R_\alpha(G)$ of G. This index has the following special cases. If $\alpha = -\frac{1}{2}$, we get the Randić index $R_{-\frac{1}{2}}(G)$. If $\alpha = 1$, we have the second Zagreb index $R_1(G)$. If $\alpha = -1$, we obtain the second modified Zagreb index $R_{-1}(G)$.
- If $f(d_x, d_y) = (d_x + d_y)^\alpha$, then $I(G)$ is the general sum-connectivity index $X_\alpha(G)$ of G. Three special cases of this index are the sum-connectivity index $X_{-\frac{1}{2}}(G)$ for $\alpha = -\frac{1}{2}$, the first Zagreb index $X_1(G)$ for $\alpha = 1$ and the hyper-Zagreb index $X_2(G)$ for $\alpha = 2$.
- If $f(d_x, d_y) = d_x^\alpha d_y^\beta + d_y^\alpha d_x^\beta$, where $\alpha, \beta \in \mathbb{R}$, then $I(G)$ is the generalized Zagreb index $GZ(G)$ of G.
- If $f(d_x, d_y) = \frac{2}{d_x + d_y}$, $I(G)$ is the harmonic index $H(G)$.
- If $f(d_x, d_y) = \frac{\sqrt{d_x d_y}}{\frac{1}{2}(d_x + d_y)}$, we get the geometric-arithmetic index $GA(G)$.
- If $f(d_x, d_y) = \frac{d_x^2 + d_y^2}{d_x d_y}$, we get the symmetric division deg index $SDD(G)$.
- If $f(d_x, d_y) = \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}$, $I(G)$ is the atom-bond connectivity index $ABC(G)$.
- If $f(d_x, d_y) = \left(\frac{d_x d_y}{d_x + d_y - 2}\right)^3$, we get the augmented Zagreb index $AZI(G)$.
- If $f(d_x, d_y) = \frac{1}{max\{d_x, d_y\}}$, $I(G)$ is the variation of the Randić index $R'(G)$.
- If $f(d_x, d_y) = \frac{d_x + d_y}{d_x d_y}$, we get the first redefined Zagreb index $ReZG_1(G)$ of G.
- If $f(d_x, d_y) = \frac{d_x d_y}{d_x + d_y}$, we obtain the second redefined Zagreb index $ReZG_2(G)$ of G.
- If $f(d_x, d_y) = d_x d_y (d_x + d_y)$, we get the third redefined Zagreb index $ReZG_3(G)$ of G.

2. **Results**

The lattice of the $TiO_2[m, n]$ nanotube for $m = 5$ and $n = 4$ is given in Fig. 1. The number of octagons in each column and row is m and n, respectively. Note that n is always even.

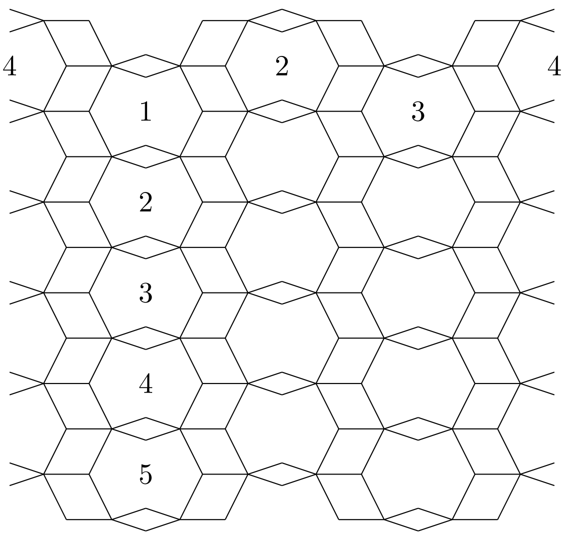

Fig. 1. $TiO_2[m,n]$ nanotube for $m=5$ and $n=4$.

The main result of this paper is the formula

$$I(TiO_2[m,n]) = [(3m-1)\cdot f(5,3) + (2m+1)\cdot f(5,2) + f(4,3) + 3\cdot f(4,2)]2n$$

for titania nanotubes $TiO_2[m,n]$. This formula can be applied to obtain any degree-based index.

The values of the most famous indices based on degrees for titania nanotubes are presented below. We do not include the names of indices, only the notations, since the names are included in the previous section. For the titania nanotube $TiO_2[m,n]$ denoted by G, we have

$$\begin{aligned}
R_\alpha(G) &= [(3m-1)15^\alpha + (2m+1)10^\alpha + 12^\alpha + 3\cdot 8^\alpha]2n,\\
R_{-\frac{1}{2}}(G) &= \frac{2(\sqrt{15}+\sqrt{10})mn}{5} + \Big(\frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{3\sqrt{2}}{2} - \frac{2\sqrt{15}}{15}\Big)n,\\
R_1(G) &= (65m+31)2n,\ R_{-1}(G) \ = \ \Big(\frac{4m}{5} + \frac{59}{60}\Big)n,\\
X_\alpha(G) &= [(3m-1)8^\alpha + (2m+2)7^\alpha + 3\cdot 6^\alpha]2n,\\
X_{-\frac{1}{2}}(G) &= \Big(\frac{3\sqrt{2}}{2} + \frac{4\sqrt{7}}{7}\Big)mn + \Big(\frac{4\sqrt{7}}{7} + \sqrt{6} - \frac{\sqrt{2}}{2}\Big)n,\\
X_1(G) &= (19m+12)4n,\ X_2(G) \ = \ (145m+71)4n,\\
GZ(G) &= [(3m-1)(5^\alpha 3^\beta + 3^\alpha 5^\beta) + (2m+1)(5^\alpha 2^\beta + 2^\alpha 5^\beta) +\\
&\quad 4^\alpha 3^\beta + 3^\alpha 4^\beta + 3(2^{2\alpha+\beta} + 2^{\alpha+2\beta})]2n,\\
H(G) &= \frac{37(m+1)n}{14},\\
GA(G) &= \Big[\frac{\sqrt{15}(3m-1)}{2} + \frac{4\sqrt{10}(2m+1)}{7} + \frac{4\sqrt{12}}{7} + 2\sqrt{8}\Big]n,
\end{aligned}$$

$$
\begin{aligned}
SDD(G) &= \frac{(756m+613)n}{30},\\
ABC(G) &= \Big[\frac{2\sqrt{10}(3m-1)}{5} + \sqrt{2}(2m+1) + \frac{\sqrt{15}}{3} + 3\sqrt{2}\Big]n,\\
AZI(G) &= \Big(\frac{503m}{4} + \frac{30199}{50}\Big)n,\\
R'(G) &= 2(m+1)n,\\
ReZG_1(G) &= 6(m+1)n,\ ReZG_2(G) = \frac{(95m+59)5n}{28},\\
ReZG_3(G) &= (250m+89)4n.
\end{aligned}
$$

3. **Proof and computations**

We prove Theorem 3.1 which contains the general formula for titania nanotubes.

Theorem 3.1. *Let G be the titania nanotube $TiO_2[m,n]$. Then*

$$I(G) = [(3m-1)\cdot f(5,3) + (2m+1)\cdot f(5,2) + f(4,3) + 3\cdot f(4,2)]2n.$$

Proof. This nanotube contains $(m+1)6n$ vertices and $(5m+4)2n$ edges. The vertices of G can be divided into the sets $V_i = \{x \in V(G) \mid d_x = i\}$ for $i = 2,3,4,5$. So V_i contains the vertices of degree i. Note that $V(G) = V_2 \cup V_3 \cup V_4 \cup V_5$. From Fig. 2 we get

$$|V_5| = 2mn,\ |V_4| = 2n,\ |V_3| = 2mn,\ |V_2| = (m+2)2n.$$

Let $E_{i,j} = \{xy \in E(G) \mid d_x = i,\ d_y = j\}$. So, $E_{i,j}$ contains the edges incident with the vertices having degrees i and j, respectively. Then

$$|E_{4,2}| = 6n,\ |E_{4,3}| = 2n,\ |E_{5,2}| = (2m+1)2n,\ |E_{5,3}| = (3m-1)2n$$

and $E(G) = E_{4,2} \cup E_{4,3} \cup E_{5,2} \cup E_{5,3}$. Then

$$
\begin{aligned}
I(G) &= \sum_{xy\in E(G)} f(d_x,d_y)\\
&= \sum_{xy\in E_{5,3}} f(5,3) + \sum_{xy\in E_{5,2}} f(5,2) + \sum_{xy\in E_{4,3}} f(4,3) + \sum_{xy\in E_{4,2}} f(4,2)\\
&= (3m-1)2n\cdot f(5,3) + (2m+1)2n\cdot f(5,2) + 2n\cdot f(4,3) +\\
&\quad 6n\cdot f(4,2)\\
&= [(3m-1)\cdot f(5,3) + (2m+1)\cdot f(5,2) + f(4,3) + 3\cdot f(4,2)]2n.
\end{aligned}
$$

□

We compute the values of the most famous indices for the titania nanotube $TiO_2[m,n]$ which is denoted by G,

For the R_α index, we get $f(d_x,d_y) = (d_xd_y)^\alpha$. So $f(5,3) = 15^\alpha$, $f(5,2) = 10^\alpha$, $f(4,3) = 12^\alpha$ and $f(4,2) = 8^\alpha$. Thus by Theorem 3.1,

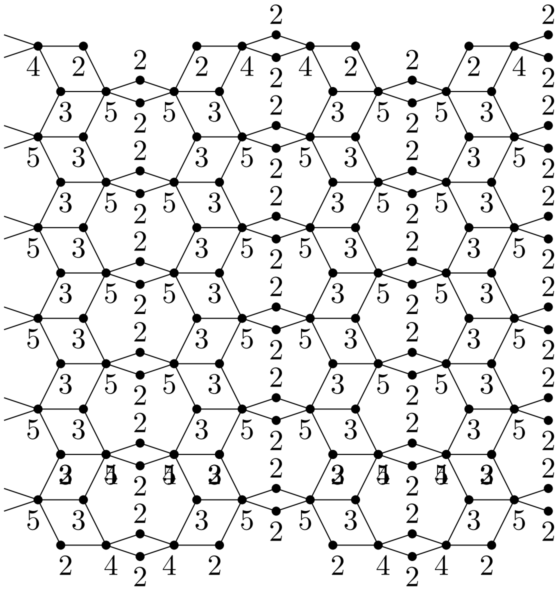

Fig. 2. $TiO_2[5,4]$ nanotube describing degrees of the vertices.

$$R_\alpha(G) = [(3m-1)\cdot 15^\alpha + (2m+1)\cdot 10^\alpha + 12^\alpha + 3\cdot 8^\alpha]2n.$$

If $\alpha = -\frac{1}{2}$, we get

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \Big(\frac{3m-1}{\sqrt{15}} + \frac{2m+1}{\sqrt{10}} + \frac{1}{\sqrt{12}} + \frac{3}{\sqrt{8}}\Big)2n \\ &= \frac{2(\sqrt{15}+\sqrt{10})mn}{5} + \Big(\frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{3\sqrt{2}}{2} - \frac{2\sqrt{15}}{15}\Big)n. \end{aligned}$$

If $\alpha = 1$, then

$$R_1(G) = [(3m-1)\cdot 15 + (2m+1)\cdot 10 + 12 + 3\cdot 8]2n = (65m+31)2n.$$

If $\alpha = -1$, then

$$R_{-1}(G) = \Big(\frac{3m-1}{15} + \frac{2m+1}{10} + \frac{1}{12} + \frac{3}{8}\Big)2n = \Big(\frac{4m}{5} + \frac{59}{60}\Big)n.$$

For the X_α index of G, we get $f(d_x,d_y) = (d_x+d_y)^\alpha$, so $f(5,3) = 8^\alpha$, $f(5,2) = 7^\alpha$, $f(4,3) = 7^\alpha$ and $f(4,2) = 6^\alpha$. So by Theorem 3.1,

$$\begin{aligned} X_\alpha(G) &= [(3m-1)\cdot 8^\alpha + (2m+1)\cdot 7^\alpha + 7^\alpha + 3\cdot 6^\alpha]2n \\ &= [(3m-1)8^\alpha + (2m+2)7^\alpha + 3\cdot 6^\alpha]2n. \end{aligned}$$

If $\alpha = -\frac{1}{2}$, we obtain

$$\begin{aligned} X_{-\frac{1}{2}}(G) &= \Big(\frac{3m-1}{\sqrt{8}} + \frac{2m+2}{\sqrt{7}} + \frac{3}{\sqrt{6}}\Big)2n \\ &= \Big(\frac{3\sqrt{2}}{2} + \frac{4\sqrt{7}}{7}\Big)mn + \Big(\frac{4\sqrt{7}}{7} + \sqrt{6} - \frac{\sqrt{2}}{2}\Big)n. \end{aligned}$$

If $\alpha = 1$, we get

$$X_1(G) = [(3m-1)8 + (2m+2)7 + 3 \cdot 6]2n = (19m+12)4n.$$

If $\alpha = 2$, then

$$X_2(G) = [(3m-1)8^2 + (2m+2)7^2 + 3 \cdot 6^2]2n = (145m+71)4n.$$

For the GZ index of G, we get $f(d_x, d_y) = d_x^\alpha d_y^\beta + d_y^\alpha d_x^\beta$, therefore $f(5,3) = 5^\alpha 3^\beta + 3^\alpha 5^\beta$, $f(5,2) = 5^\alpha 2^\beta + 2^\alpha 5^\beta$, $f(4,3) = 4^\alpha 3^\beta + 3^\alpha 4^\beta$ and $f(4,2) = 4^\alpha 2^\beta + 2^\alpha 4^\beta = 2^{2\alpha+\beta} + 2^{\alpha+2\beta}$. Thus by Theorem 3.1,

$$\begin{aligned} GZ(G) &= [(3m-1)(5^\alpha 3^\beta + 3^\alpha 5^\beta) + (2m+1)(5^\alpha 2^\beta + 2^\alpha 5^\beta) + \\ &\quad 4^\alpha 3^\beta + 3^\alpha 4^\beta + 3(2^{2\alpha+\beta} + 2^{\alpha+2\beta})]2n. \end{aligned}$$

For the H index, we get $f(d_x, d_y) = \frac{2}{d_x+d_y}$, thus $f(5,3) = \frac{2}{8} = \frac{1}{4}$, $f(5,2) = \frac{2}{7}$, $f(4,3) = \frac{2}{7}$ and $f(4,2) = \frac{2}{6} = \frac{1}{3}$. Therefore

$$H(G) = \Big[(3m-1) \cdot \frac{1}{4} + (2m+1) \cdot \frac{2}{7} + \frac{2}{7} + 3 \cdot \frac{1}{3}\Big]2n = \frac{37(m+1)n}{14}.$$

For the GA index of G, we obtain $f(d_x, d_y) = \frac{\sqrt{d_x d_y}}{\frac{1}{2}(d_x+d_y)}$, thus $f(5,3) = \frac{\sqrt{15}}{4}$, $f(5,2) = \frac{2\sqrt{10}}{7}$, $f(4,3) = \frac{2\sqrt{12}}{7}$ and $f(4,2) = \frac{\sqrt{8}}{3}$. Then by Theorem 3.1,

$$\begin{aligned} GA(G) &= \Big[(3m-1) \cdot \frac{\sqrt{15}}{4} + (2m+1) \cdot \frac{2\sqrt{10}}{7} + \frac{2\sqrt{12}}{7} + 3 \cdot \frac{\sqrt{8}}{3}\Big]2n \\ &= \Big[\frac{\sqrt{15}(3m-1)}{2} + \frac{4\sqrt{10}(2m+1)}{7} + \frac{4\sqrt{12}}{7} + 2\sqrt{8}\Big]n. \end{aligned}$$

For the SDD index, we get $f(d_x, d_y) = \frac{d_x^2+d_y^2}{d_x d_y}$, thus $f(5,3) = \frac{34}{15}$, $f(5,2) = \frac{29}{10}$, $f(4,3) = \frac{25}{12}$ and $f(4,2) = \frac{20}{8} = \frac{10}{4}$. Then

$$SDD(G) = \Big[(3m-1) \cdot \frac{34}{15} + (2m+1) \cdot \frac{29}{10} + \frac{25}{12} + 3 \cdot \frac{10}{4}\Big]2n = \frac{(756m+613)n}{30}.$$

For the ABC index, we get $f(d_x, d_y) = \sqrt{\frac{d_x+d_y-2}{d_x d_y}}$, therefore $f(5,3) = \sqrt{\frac{6}{15}} = \sqrt{\frac{2}{5}}$, $f(5,2) = \sqrt{\frac{5}{10}} = \frac{1}{\sqrt{2}}$, $f(4,3) = \sqrt{\frac{5}{12}}$ and $f(4,2) = \sqrt{\frac{4}{8}} = \frac{1}{\sqrt{2}}$. Thus

$$\begin{aligned} ABC(G) &= \Big[(3m-1) \cdot \sqrt{\frac{2}{5}} + (2m+1) \cdot \frac{1}{\sqrt{2}} + \sqrt{\frac{5}{12}} + 3 \cdot \frac{1}{\sqrt{2}}\Big]2n \\ &= \Big[\frac{2\sqrt{10}(3m-1)}{5} + \sqrt{2}(2m+1) + \frac{\sqrt{15}}{3} + 3\sqrt{2}\Big]n. \end{aligned}$$

For the AZI index, we get $f(d_x, d_y) = (\frac{d_x d_y}{d_x+d_y-2})^3$, thus $f(5,3) = (\frac{15}{6})^3 = \frac{125}{8}$, $f(5,2) = (\frac{10}{5})^3 = 8$, $f(4,3) = (\frac{12}{5})^3 = \frac{1728}{125}$ and $f(4,2) = (\frac{8}{4})^3 = 8$. Then

$$AZI(G) = \Big[(3m-1) \cdot \frac{125}{8} + (2m+1) \cdot 8 + \frac{1728}{125} + 3 \cdot 8\Big]2n = \Big(\frac{503m}{4} + \frac{30199}{50}\Big)n.$$

For the R' index, we obtain $f(d_x, d_y) = \frac{1}{max\{d_x,d_y\}}$, therefore $f(5,3) = \frac{1}{5}$, $f(5,2) = \frac{1}{5}$, $f(4,3) = \frac{1}{4}$ and $f(4,2) = \frac{1}{4}$. Thus

$$R'(G) = \Big[(3m-1)\cdot\frac{1}{5} + (2m+1)\cdot\frac{1}{5} + \frac{1}{4} + 3\cdot\frac{1}{4}\Big]2n = 2(m+1)n.$$

For the $ReZG_1$ index, we get $f(d_x, d_y) = \frac{d_x+d_y}{d_x d_y}$, therefore $f(5,3) = \frac{8}{15}$, $f(5,2) = \frac{7}{10}$, $f(4,3) = \frac{7}{12}$ and $f(4,2) = \frac{6}{8} = \frac{3}{4}$. Thus

$$ReZG_1(G) = \Big[(3m-1)\cdot\frac{8}{15} + (2m+1)\cdot\frac{7}{10} + \frac{7}{12} + 3\cdot\frac{3}{4}\Big]2n = 6(m+1)n.$$

For the $ReZG_2$ index, we obtain $f(d_x, d_y) = \frac{d_x d_y}{d_x+d_y}$, so $f(5,3) = \frac{15}{8}$, $f(5,2) = \frac{10}{7}$, $f(4,3) = \frac{12}{7}$ and $f(4,2) = \frac{8}{6} = \frac{4}{3}$. Thus

$$ReZG_2(G) = \Big[(3m-1)\cdot\frac{15}{8} + (2m+1)\cdot\frac{10}{7} + \frac{12}{7} + 3\cdot\frac{4}{3}\Big]2n = \frac{(95m+59)5n}{28}.$$

For the $ReZG_3$ index, we get $f(d_x, d_y) = (d_x + d_y)d_x d_y$, so $f(5,3) = 120$, $f(5,2) = 70$, $f(4,3) = 84$ and $f(4,2) = 48$. Thus

$$ReZG_3(G) = [(3m-1)\cdot 120 + (2m+1)\cdot 70 + 84 + 3\cdot 48]2n = (250m+89)4n.$$

4. **Conclusion**

Titania nanotubes belong to the most studied compounds in materials science. We used indices of graphs to represent connections between structures and chemical properties of titania nanotubes. Vertices and edges of graphs can model titania nanotubes; see [9].

We obtained a general formula that can be applied to obtain any degree-based index (defined by the sum for the edges) for titania nanotubes. We also presented the values of the most famous indices based on degrees for titania nanotubes. For example, if $m = 5$ and $n = 4$, then from Theorem 3.1 we obtain the invariant

$$I(TiO_2[5,4]) = 112\cdot f(5,3) + 88\cdot f(5,2) + 8\cdot f(4,3) + 24\cdot f(4,2).$$

Then, using $f(d_x, d_y) = (d_x d_y)^\alpha$, $f(d_x, d_y) = (d_x + d_y)^\alpha$ and $f(d_x, d_y) = d_x^\alpha d_y^\beta + d_y^\alpha d_x^\beta$, we get the general Randić index

$$R_\alpha(TiO_2[5,4]) = 112\cdot 15^\alpha + 88\cdot 10^\alpha + 8\cdot 12^\alpha + 24\cdot 8^\alpha,$$

the general sum-connectivity index

$$X_\alpha(TiO_2[5,4]) = 112\cdot 8^\alpha + 96\cdot 7^\alpha + 24\cdot 6^\alpha$$

and the generalized Zagreb index

$$\begin{aligned} GZ(TiO_2[5,4]) &= 112(5^\alpha 3^\beta + 3^\alpha 5^\beta) + 88(5^\alpha 2^\beta + 2^\alpha 5^\beta) \\ &+ 8(4^\alpha 3^\beta + 3^\alpha 4^\beta) + 24(2^{2\alpha+\beta} + 2^{\alpha+2\beta}), \end{aligned}$$

where α and β are real numbers. These indices can be used for instance in the development of quantitative structure-activity relationships. The importance of these indices is described in detail also in [6].

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REFERENCES

[1] *A. Ahmad*, Topological properties of sodium chloride, U. P. B. Sci. Bull. Series B **82** (2020), No. 1, 35-46.

[2] *M. Bača, J. Horváthová, M. Mokrišová, A. Semaničová-Feňovčíková and A. Suhányiová*, On topological indices of carbon nanotube network, Canad. J. Chem. **93** (2015), No. 10, 1-4.

[3] *W. Gao, S. Baby, M. K. Shafiq, H. M. A. Siddiqui and M. R. Farahani*, On Randić indices of single-walled TiO_2 nanotubes, U. P. B. Sci. Bull. Series B **79** (2017), No. 1, 93-100.

[4] *W. Gao, M. R. Farahani and M. Imran*, About the Randić connectivity, modify Randić connectivity and sum-connectivity indices of titania nanotubes $TiO_2(m, n)$, Acta Chim. Slov. **64** (2017), No. 1, 256-260.

[5] *W. Gao, M. R. Farahani, M. K. Jamil and M. K. Siddiqui*, The redefined first, second and third Zagreb indices of titania nanotubes $TiO_2[m, n]$, Open Biotechnology Journal **10** (2016), 272-277.

[6] https://en.wikipedia.org/wiki/Topological_index.

[7] *Y. Huo, J.-B. Liu, M. Imran, M. Saeed, M. R. Farahani, M. A. Iqbal and M. A. Malik*, On some degree-based topological indices of line graphs of $TiO_2[m, n]$ nanotubes, J. Comput. Theor. Nanosci. **13** (2016), No. 12, 9131-9135.

[8] *M. Javaid, J.-B. Liu, M. A. Rehman and S. Wang*, On the certain topological indices of titania nanotube $TiO_2[m, n]$, Z. Naturforsch. A **72** (2017), No. 7, 647-654.

[9] *J.-B. Liu, W. Gao, M. K. Siddiqui and M. R. Farahani*, Computing three topological indices for titania nanotubes $TiO_2[m, n]$ AKCE Int. J. Graphs Comb. **13** (2017), No. 3, 255-260.

[10] *M. A. Malik and M. Imran*, On multiple Zagreb indices of TiO_2 nanotubes, Acta Chim. Slov. **62** (2015), No. 4, 973-976.

[11] *M. Munir, W. Nazeer, A. R. Nizami, S. Rafique and S. M. Kang*, M-polynomials and topological indices of titania nanotubes, Symmetry **8** (2016), No. 11, 117.

[12] *T. Vetrík*, Degree-based topological indices of hexagonal nanotubes, J. Appl. Math. Comput. **58** (2018), No. 1, 111-124.

[13] *T. Vetrík*, The Randić index and the redefined Zagreb index of titania nanotubes $TiO_2[m, n]$, U. P. B. Sci. Bull. Series B **80** (2018), No. 1, 157-162.

[14] *L. Yan, Y. Li, S. Hayat, H. M. A. Siddiqui, M. Imran, S. Ahmad and M. R. Farahani*, On degree-based and frustration related topological indices of single-walled titania nanotubes, J. Comput. Theor. Nanosci. **13** (2016), No. 11, 9027-9032.