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Scientific paper

On Eccentric Connectivity Index of TiO_2 Nanotubes

Imran Nadeem and Hani Shaker*

Department of Mathematics, COMSATS Institute of Information Technology, Defence Road, Off Raiwind Road, Lahore, Pakistan

** Corresponding author: E-mail: hani.uet@gmail.com, imran7355@gmail.com Phone: +92-42-111001007, +92-321-4120429*

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Abstract

The eccentric connectivity index (ECI) is a distance based molecular structure descriptor that was recently used for mathematical modeling of biological activities of diverse nature. The ECI has been shown to give a high degree of predictability compare to Wiener index with regard to diuretic activity and anti-inflammatory activity. The prediction accuracy rate of ECI is better than the Zagreb indices in case of anticonvulsant activity. Titania nanotubular materials are of high interest metal oxide substances due to their widespread technological applications. The numerous studies on the use of this material also require theoretical studies on the other properties of such materials. Recently, the Zagreb indices were studied of an infinite class of titania (TiO_2) nanotubes [32]. In this paper, we study the eccentric connectivity index of these nanotubes.

Keywords: TiO_2 nanotubes, Topological indices, Eccentric connectivity index

1. Introduction

Cheminformatics is a new subject which is a combination of chemistry, mathematics and information science. It studies quantitative structure activity relationships (QSAR) and structure property relationships (QSPR) that are used to predict the biological activities and properties of chemical compounds. In the QSAR/QSPR study, physicochemical properties and topological indices are used to predict biological activity of the chemical compounds.

A topological index is a numerical descriptor of the molecular structure based on certain topological features of the corresponding molecular graph. Topological indices are graph invariant and are a convenient means of translating chemical constitution into numerical values which can be used for correlation with physical properties in QSPR/QSAR studies.[1–3] Topological indices are also used as a measure of structural similarity or diversity and thus they may give a measure of the diversity of chemical databases. There are two major classes of topological indices such as distance based topological indices and degree based topological indices. Among these classes, distance based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry.

A graph G with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a path between any pair of vertices in G. The degree of a vertex $u \in V$ is the number of edges incident to u and denoted by $deg(u)$. For two vertices u, v of a graph G their distance $d(u, v)$ is defined as the length of any shortest path connecting u and v in G. For a given vertex u of G its eccentricity $\varepsilon(u)$ is the largest distance between u and any vertex v of G.

Sharma et al.[9] introduced a distance based topological index, the eccentric connectivity index (ECI) $\xi^c(G)$ of G, defined as

$$\xi^c(G) = \sum_{v \in V(G)} deg(v)\,\varepsilon(v) \qquad (1)$$

It is reported in[4–8] that ECI provides excellent correlations with regard to both physical and biological properties. The eccentric connectivity index is successfully used for mathematical models of biological activities of diverse nature. The simplicity amalgamated with high correlating ability of this index can easily be exploited in QSPR/QSAR studies.[9–11] The prediction accuracy rate of ECI is better than the Wiener index with regard to diuretic activity[12] and anti-inflammatory activity.[13] Compare to Zagreb indices, the ECI has been shown to give a high degree of predictability in case of anticonvulsant activity.[14] Recently, the eccentric connectivity index was studied for certain nanotubes[15–19] and for various classes of graphs.[20–22]

The titanium nanotubular materials, called titania by a generic name, are of high interest metal oxide substances due to their widespread applications in production of catalytic, gas-sensing and corrosionresistance materials.[23] As a well-known semiconductor with numerous technological applications, Titania (TiO_2) nanotubes are comprehensively studied in materials science.[24] The TiO_2 nanotubes were systematically synthesized using different methods[25] and carefully studied as prospective technological materials. Theoretical studies on the stability and electronic characteristics of titania nanostructures have extensively been studied.[26–28] The numerous studies on the use of titania in technological applications also required theoretical studies on stability and other properties of such structures.[29–31]

Recently, M. A. Malik et al.[32] studied the Zagreb indices of an infinite class of TiO_2 nanotubes. In this paper, we study eccentric connectivity index of these nanotubes.

2. Main Results

The molecular graph of titania nanotubes $TiO_2[m,n]$ is presented in Figure 1, where m denotes the number of octagons in a row and n denotes the number of octagons in a column of the titania nanotube.

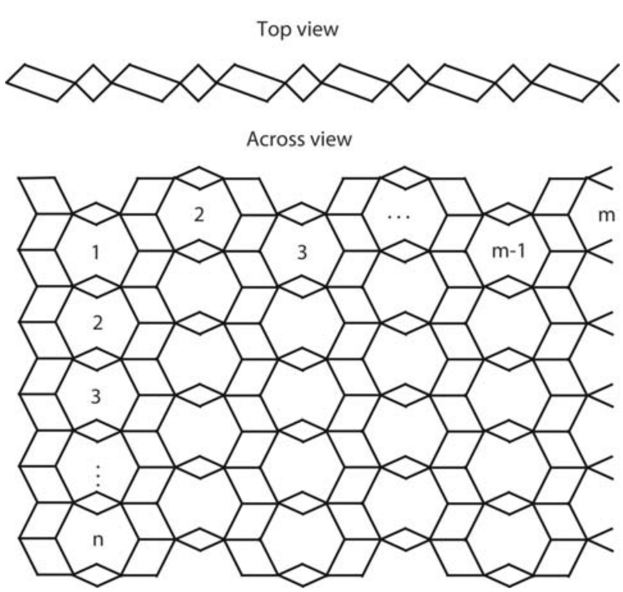

Figure 1: The molecular graph of TiO_2[m,n] nanotube.

The molecular graph of $TiO_2[m,n]$ nanotube has $2n+2$ rows and m columns. For each i^{th} row and j^{th} column, we label the vertices of $TiO_2[m,n]$ nanotube by u_{ij}, v_{ij}, x_{ij} and y_{ij} as shown in Figure 2.

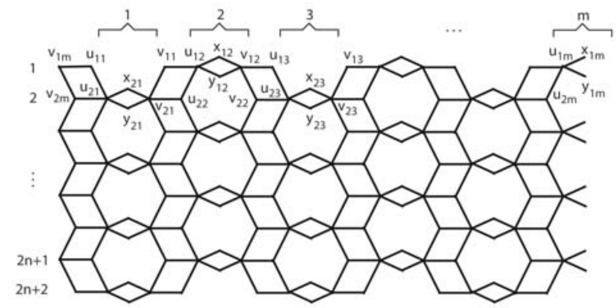

Figure 2: The labeled vertices of TiO_2[m,n] nanotube.

In the molecular graph, G, of TiO_2 nanotubes, we can see that $2 \leq deg(v) \leq 5$. So, we have the vertex partitions as follows.

$$V_1 = \{v \in V(G) \mid deg(v) = 2\}, \quad V_2 = \{v \in V(G) \mid deg(v) = 3\}$$
$$V_3 = \{v \in V(G) \mid deg(v) = 4\}, \quad V_4 = \{v \in V(G) \mid deg(v) = 5\} \tag{2}$$

The cardinalities of all vertex partitions are presented in Table 1.

Table 1: The vertex partitions of the TiO_2 nanotubes along with their cardinalities.

Vertex partition	Cardinality
V_1	$2mn + 4m$
V_2	$2mn$
V_3	$2m$
V_4	$2mn$

In the following, we compute the exact formulas for eccentric connectivity index of $TiO_2[m,n]$ nanotubes.

Theorem 2.1 *Let $TiO_2[m,n]$ be the graph of titania nanotube, then for* $n \leq \left\lfloor \frac{m-2}{4} \right\rfloor$ *we have*

$$\xi^c(TiO_2[m,n]) = 40m^2n + 32m^2 \tag{3}$$

Proof. Consider $G = TiO_2[m,n]$. When $n \leq \left\lfloor \frac{m-2}{4} \right\rfloor$, the eccentricity of every vertex in every row is $2m$. From Table 1, we have

$$\begin{aligned} \xi^c(G) &= \sum_{v \in V(G)} \deg(v)\varepsilon(v) \\ &= (2mn+2m)(2)(2m) + (2m)(2)(2m) + \\ &\quad + (2mn)(3)(2m) + (2m)(4)(2m) + (2mn)(5)(2m) \\ &= 40m^2n + 32m^2. \end{aligned} \tag{4}$$

Theorem 2.2 *Let $TiO_2[m,n]$ be the graph of titania nanotube, where $m = 2p$ then for p even we have*

$$\xi^c\left(TiO_2[m,n]\right)=\begin{cases}160p^2n+48pn+104p^2+24p & \text{if } p=2n;\\ 28p^3+48p^2n+112pn^2+128pn+64p^2+24p & \text{if } \frac{p-2}{2}<n<p-1 \text{ and } p\neq 2n;\\ 120p^2n+68pn^2+112pn+96p^2+52p & \text{if } n\geq p-1 \text{ and } n \text{ is odd};\\ 120p^2n+60pn^2+72pn+104p^2+24p & \text{if } n>p-1 \text{ and } n \text{ is even}.\end{cases} \tag{5}$$

Proof. Consider $G = TiO_2[m,n]$. With respect to the eccentricity of vertices, we have the following cases.

Case 1. When $p = 2n$

In this case the eccentricity of the vertices u_{ij}, v_{ij} is $3p + 2n + 1$ where $i = 1,2n + 2$. The eccentricity of each vertex in the remaining $2n$ rows is $4p$. Hence

$$\begin{aligned}\xi^c(G)&=\sum_{v\in V(G)}\deg(v)\varepsilon(v)\\ &=2(2p)(2)(3p+2n+1)+2(2p)(4)(3p+2n+1)+(2p)(2n)(3)(4p)+(2p)(2n)(5)(4p)+2p(2n+2)(2)(4p)\\ &=160p^2n+48pn+104p^2+24p.\end{aligned} \tag{6}$$

Case 2. when $\frac{p-2}{2}<n<p-1$ and $p\neq 2n$

In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3-i)j}$, $v_{(2n+3-i)j}$. where $i = 1,2, \cdots, 2n - p + 1$. The eccentricity of these vertices in i^{th} row is given by

$$\begin{aligned}&\varepsilon(u_{ij})=\varepsilon(v_{ij})=3p+2n+2-i\\ &\text{where } i=1,2,\cdots,2n-p+1\end{aligned} \tag{7}$$

The eccentricity of vertices u_{ij}, v_{ij} in remaining $2p - 2n$ rows is $4p$.

Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3i)j}$, $y_{(2n+3-i)j}$, $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$ where $i = 1,2, \cdots, (2n - p)/2$. The eccentricity of these vertices in i^{th} row is given by

$$\begin{aligned}&\varepsilon(x_{ij})=\varepsilon(y_{ij})=3p+2n+2-2i\\ &\text{where } i=1,2,\cdots,(2n-p)/2\end{aligned} \tag{8}$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining $(2p - 2n + 2)$ rows is $4p$. Hence

$$\begin{aligned}\xi^c(G)&=\sum_{v\in V(G)}\deg(v)\varepsilon(v)\\ &=2(2p)(2)(3p+2n+1)+2(2p)(4)(3p+2n+1)+2(2p)(3)\sum_{i=2}^{2n-p+1}(3p+2n+2-i)\\ &\quad+2(2p)(5)\sum_{i=2}^{2n-p+1}(3p+2n+2-i)+(2p)(2p-2n)(3)(4p)+(2p)(2p-2n)(5)(4p)\\ &\quad+4(2p)(2)\sum_{i=1}^{(2n-p)/2}(3p+2n+2-2i)+(2p)(2p-2n+2)(2)(4p)\\ &=28p^3+48p^2n+112pn^2+128pn+64p^2+24p\end{aligned} \tag{9}$$

Case 3. When $n \geq p - 1$ and n is odd

In this case the eccentricity of vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3-i)j}$, $v_{(2n+3-i)j}$ where $i = 1,2, \cdots, n + 1$. The eccentricity of these vertices in i^{th} row is given by

$$\begin{aligned}&\varepsilon(u_{ij})=\varepsilon(v_{ij})=3p+2n+2-i\\ &\text{where } i=1,2,\cdots,n+1\end{aligned} \tag{10}$$

Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3i)j}$, $y_{(2n+3-i)j}$, $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$ where $i = 1,2, \cdots, (n + 1)/2$. The eccentricity of these vertices in i^{th} row is given by

$$\begin{aligned}&\varepsilon(x_{ij})=\varepsilon(y_{ij})=3p+2n+2-2i\\ &\text{where } i=1,2,\cdots,(n+1)/2\end{aligned} \tag{11}$$

The shortest paths having maximal length in $TiO_2[8,7]$ nanotube are shown in Figure 3.

Hence

$$\begin{aligned}\xi^c(G)&=\sum_{v\in V(G)}\deg(v)\varepsilon(v)\\ &=2(2p)(2)(3p+2n+1)+2(2p)(4)(3p+2n+1)+\\ &\quad+2(2p)(3)\sum_{i=2}^{n+1}(3p+2n+2-i)\\ &\quad+2(2p)(5)\sum_{i=2}^{n+1}(3p+2n+2-i)+4(2p)(2)\\ &\quad\sum_{i=1}^{(n+1)/2}(3p+2n+2-2i)\\ &=120p^2n+68pn^2+112pn+96p^2+52p\end{aligned} \tag{12}$$

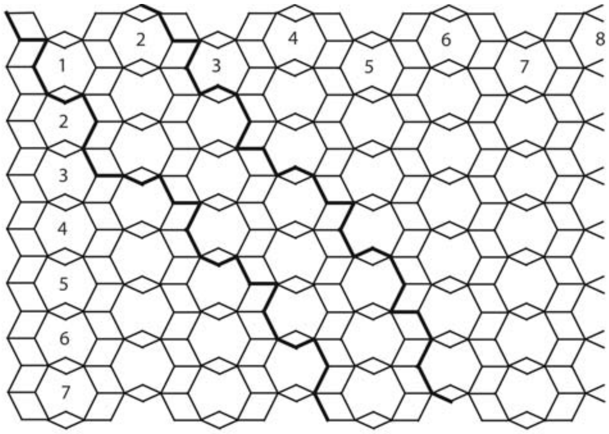

Figure 3: The shortest paths having maximal length in $TiO_2[8,7]$ nanotube.

Case 4. When $n > p - 1$ and n is even

In this case the eccentricity of vertices u_{ij}, v_{ij} is same as we discussed in case 3. Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3-i)j}$, $y_{(2n+3-i)j}$, $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$ where $i = 1,2, \cdots, n/2$. The eccentricity of these vertices in i^{th} row is given by

$$\begin{gathered}\varepsilon(x_{ij}) = \varepsilon(y_{ij}) = 3p+2n+2-2i \\ \text{where } i=1,2,\cdots,n/2\end{gathered} \tag{13}$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining 2 rows is $4p$. Hence

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} \deg(v)\varepsilon(v) \\ &= 2(2p)(2)(3p+2n+1)+2(2p)(4)(3p+2n+1)+ \\ &\quad +2(2p)(3)\sum_{i=2}^{n+1}(3p+2n+2-i) \\ &\quad +2(2p)(5)\sum_{i=2}^{n+1}(3p+2n+2-i)+4(2p)(2) \\ &\quad \sum_{i=1}^{n/2}(3p+2n+2-2i)+2(2p)(2)(4p) \\ &= 120p^2n+60pn^2+72pn+104p^2+24p\end{aligned} \tag{14}$$

Theorem 2.3 *Let $TiO_2[m,n]$ be the graph of titania nanotube, where $m = 2p$ then for p odd we have*

$$\xi^c\left(TiO_2[m,n]\right)=\begin{cases}160p^2n+128pn+192p^2+32p & \text{if } p=2n-1; \\ 20p^3+80p^2n+80pn^2+96pn+80p^2+28p & \text{if } \dfrac{p-1}{2}<n<p-1 \text{ and } p\neq 2n-1; \\ 120p^2n+60pn^2+72pn+72p^2+28p & \text{if } n>p-1 \text{ and } n \text{ is odd}; \\ 120p^2n+60pn^2+80pn+96p^2+32p & \text{if } n\geq p-1 \text{ and } n \text{ is even.}\end{cases} \tag{15}$$

Proof. Consider $G = TiO_2[m,n]$. With respect to the eccentricity of vertices, we have the following cases.

Case 1. When $p = 2n - 1$

In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3-i)j}$, $v_{(2n+3-i)j}$, where $i = 1,2$. The eccentricity of these vertices in i^{th} row is given by

$$\varepsilon(u_{ij}) = \varepsilon(v_{ij}) = 3p+2n+2-i \quad \text{where } i=1,2 \tag{16}$$

The eccentricity of vertices u_{ij}, v_{ij} in remaining $2n$ rows is $4p$. Also, the eccentricity of the vertices x_{1j}, y_{1j} is same as the eccentricity of vertices $x_{(2n+2)j}$, $x_{(2n+2)j}$. The eccentricity of the vertices x_{1j}, y_{1j} is given by

$$\varepsilon(x_{1j}) = \varepsilon(y_{1j}) = 3p+2n+1 \tag{17}$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining $2n$ rows is $4p$. The shortest paths having maximal length in $TiO_2[14,4]$ nanotube are shown in Figure 4.

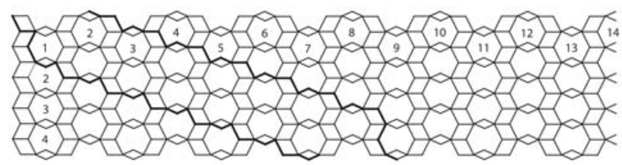

Figure 4: The shortest paths having maximal length in $TiO_2[14,4]$ nanotube.

Hence

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} \deg(v)\varepsilon(v) \\ &= 2(2p)(2)(3p+2n+1)+2(2p)(4)(3p+2n+1)+ \\ &\quad +2(2p)(3)(3p+2n)+2(2p)(5)(3p+2n) \\ &\quad +(2p)(2n)(3)(4p)+(2p)(2n)(5)(4p)+ \\ &\quad +2(2p)(2)(3p+2n+1)+(2p)(2n)(2)(4p) \\ &= 160p^2n+128pn+192p^2+32p\end{aligned} \tag{18}$$

Case 2. when $\frac{p-1}{2} < n < p-1$ and $p \neq 2n-1$

In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as we discussed in Case 2 of Theorem 2.2. The eccentricity of the vertices x_{1j}, y_{1j}, $x_{(2n+2)j}$, $x_{(2n+2)j}$ is same as we discussed in Case 1.

Also, the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$, $x_{(2n+1-i)j}$, $y_{(2n+1-i)j}$ where $i = 1,2, \cdots, (2n - p - 1)/2$. The eccentricity of these vertices in $(i + 1)^{th}$ row is given by

$$\varepsilon(x_{(i+1)j}) = \varepsilon(y_{(i+1)j}) = 3p + 2n + 1 - 2i \quad \text{where } i = 1,2,\cdots,(2n-p-1)/2 \tag{19}$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining $(2p - 2n + 2)$ rows is $4p$. Hence

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} \deg(v)\varepsilon(v)\\ &= 2(2p)(2)(3p+2n+1) + 2(2p)(4)(3p+2n+1) + 2(2p)(3)\sum_{i=2}^{2n-p+1}(3p+2n+2-i)\\ &\quad +2(2p)(5)\sum_{i=2}^{2n-p+1}(3p+2n+2-i) + (2p)(2p-2n)(3)(4p) + (2p)(2p-2n)(5)(4p)\\ &\quad +2(2p)(2)(3p+2n+1) + 4(2p)(2)\sum_{i=1}^{(2n-p-1)/2}(3p+2n+1-2i) + 2p(2p-2n+2)(2)(4p)\\ &= 20p^3 + 80p^2n + 80pn^2 + 96pn + 80p^2 + 28p\end{aligned} \tag{20}$$

Case 3. When $n > p - 1$ and n is odd

In this case the eccentricity of the vertices u_{ij}, v_{ij}, x_{1j}, y_{1j}, $x_{(2n+2)j}$, $x_{(2n+2)j}$ is same as we discussed in Case 2. Also, the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$, $x_{(2n+1-i)j}$, $y_{(2n+1-i)j}$ where $i = 1,2, \cdots, (n - 1)/2$. The eccentricity of these vertices in $(i + 1)^{th}$ row is given by

$$\varepsilon(x_{i+1}) = \varepsilon(y_{i+1}) = 3p + 2n + 1 - 2i \quad \text{where } i = 1,2,\cdots,(n-1)/2 \tag{21}$$

Hence

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} \deg(v)\varepsilon(v)\\ &= 2(2p)(2)(3p+2n+1) + 2(2p)(4)(3p+2n+1) + 2(2p)(3)\sum_{i=2}^{n+1}(3p+2n+2-i)\\ &\quad +2(2p)(5)\sum_{i=2}^{n+1}(3p+2n+2-i) + 2(2p)(2)(3p+2n+1) + 4(2p)(2)\sum_{i=1}^{(n-1)/2}(3p+2n+1-2i)\\ &= 120p^2n + 60pn^2 + 72pn + 72p^2 + 28p\end{aligned} \tag{22}$$

Case 4. When $n \geq n - 1$ and n is even.

In this case the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2-i)j}$, $y_{(2n+2-i)j}$, $x_{(2n+1-i)j}$, $y_{(2n+1-i)j}$ where $i = 1,2, \cdots, n/2$. The eccentricity of these vertices in $(i + 1)^{th}$ row is given by

$$\varepsilon(x_{i+1}) = \varepsilon(y_{i+1}) = 3p + 2n + 1 - 2i \quad \text{where } i = 1,2,\cdots,n/2 \tag{23}$$

The eccentricity of the remaining vertices is same as we discussed in case 3.

Hence

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} \deg(v)\varepsilon(v)\\ &= 2(2p)(2)(3p+2n+1) + 2(2p)(4)(3p+2n+1) +\\ &\quad + 2(2p)(3)\sum_{i=2}^{n+1}(3p+2n+2-i)\\ &\quad +2(2p)(5)\sum_{i=2}^{n+1}(3p+2n+2-i) + 2(2p)(2)\\ &\quad (3p+2n+1) + 4(2p)(2)\sum_{i=1}^{n/2}(3p+2n+1-2i)\\ &= 120p^2n + 60pn^2 + 80pn + 96p^2 + 32p\end{aligned} \tag{24}$$

3. Conclusion

The eccentric connectivity index provides excellent prediction accuracy rate compare to other indices in certain biological activities of diverse nature such as diuretic activity, anticonvulsant activity and anti-inflammatory activity. In this sense, this index is very useful in QSPR/QSAR studies. In this paper, we study eccentric connectivity index of an infinite class of TiO_2 nanotubes. By using this index, we can find mathematical models of certain biological activities for this material. With the help of these models, we can predict about certain biological activities for this material.

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Povzetek

Med molekulske strukturne deskriptorje spada tudi »eccentric connectivity« indeks (ECI), ki je bil pred kratkim uporabljen za matematično modeliranje raznovrstnih bioloških aktivnosti. V primerjavi z Wienerjevim indeksom, daje ECI visoko stopnjo predvidljivosti v primeru diuretične in protivnetne aktivnosti. Stopnja natančnosti napovedi indeksa ECI je boljša od zagebškega indeksa v primeru antikonvulzivne aktivnosti. Med kovinskimi oksidi predstavljajo nanocevke TiO_2 material, ki ima veliko tehnološko uporabnost. Številne študije tega materiala zahtevajo tudi teoretične študije njegovih lastnosti. Nedavno je bil za nanocevke TiO_2 določen zagrebški indeks, v tem prispevku pa preučujemo indeks ECI.