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ON RANDIĆ INDICES OF SINGLE-WALLED TiO_2 NANOTUBES

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In mathematical chemistry several topological indices have been introduced that can be classified as: (i). distance-based topological indices and (ii). degree-based topological indices. Each index measures some specific property of the molecular structure. In QSAR study, physico-chemical properties and topological indices such as Zagreb, Randić, ABC indices are used to predict the bioactivity of chemical compounds. Graph theory plays a vital role in this area of research. In this paper we present the formulas of general Randić, reduced Randić and reduced reciprocal Randić indices for two types of single-walled titania nanotubes (SW TiO_2 NTs) based on their structural layers in underlying chemical structure: 3-layered SW TiO_2 NTs and 6-layered SW TiO_2 NTs.

Keywords: TiO_2 nanotubes, Topological indices, Randić index, Reduced Randić index, Reduced reciprocal Randić index

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1. Introduction

The branch of chemistry in which we discuss and predict the molecular properties by using mathematical tools without referring to quantum mechanics is called mathematical chemistry [1,2]. The branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena is known as chemical graph theory [2]. This theory is much beneficial in the development of the chemical sciences.

A molecular graph is a simple graph in which we show atoms by vertices

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and chemical bonds between these atoms by edges, where the hydrogen atoms are often omitted. Let G be a molecular graph with vertex set V(G) and edge set E(G). The cardinalities of the sets V(G) and E(G) are called order and size of G, respectively. An edge in E(G) with end vertices u and v is denoted by uv. The vertices having an edge between them are called adjacent vertices. The set of all vertices adjacent to the vertex u is called the neighborhood of u and is denoted by N(u). The degree of u in G is defined as the cardinality of N(u) and is denoted by $d_u(G)$.

These indices describe the structure and the branching pattern of the molecule numerically. So, the topological analysis of a molecule assigns unique number (index) to the structure of the molecule. This unique number may be considered as descriptor of the molecule under observation. The topological indices play a significant role in quantitative structure-activity research (QSAR) and structure-property relationships research (QSPR) study. In the QSAR study, topological indices such as Zagreb index, Wiener index, Szeged index, Randić index and ABC index are used to predict bioactivity of the chemical compounds.

Titania (TiO_2) is one of the most comprehensively studied metal oxide substances due to its wide spread applications in production of catalytic, gas-sensing and corrosion-resistance materials [3]. TiO_2 attracts considerable technological interest due to unique properties in biology, optics, electronics and photo-chemistry [4]. Recent experimental studies show that titania nanotubes (TiO_2 NTs) improve TiO_2 bulk properties for photocatalysis, hydrogen-sensing and photo-voltaic applications [5]. TiO_2 NTs have been fabricated by a number of different methods, such as hydrothermal treatment, template-assistant deposition and others. Various TiO_2 NTs were observed in two types of morphologies: multi-walled (MW) cylindrical and scroll-like frequently containing various types of defects and impurities [6].

Although the first vertex-degree-based structure descriptors were the graph invarients that are known as first and second Zagreb indices [7, 8]. But these were used for a different purpose and were included among topological indices in 1983 by Balaban et al. [9]. However, the first genuine degree-based topological index was put forward in 1975 by Milan Randić [10]. His index was defined as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u(G) d_v(G)}}$$

Randić himself named it,“ branching index" but soon it was re-named,“ connectivity index" [11, 12]. Now it is reffered as, “Randić index". It is the fact that Randić index is the most studied, most often applied and most popular among all topological indices. The number of papers devoted to this graph invariant is in hundreds. A few books are also written on this structure descriptor. The suitability of the Randić index for drug design was recognized [8, 10] and the index was used for this purpose. The general Randić index was proposed by Bollobás [13] and Amic et al. [14] independently, in 1998 and was defined as

$$R_\alpha(G) = \sum_{uv\in E(G)}(d_u(G)d_v(G))^\alpha, \text{ where } \alpha \text{ is a variable parameter.}$$

The reciprocal Randić index is defined as

$$RR = RR(G) = \sum_{uv\in E(G)}\sqrt{d_u(G)d_v(G)}$$

It is of course a special case of the much examined, " general Randić index" $R_\alpha(G) = \sum_{uv\in E(G)}(d_u(G)d_v(G))^\alpha$, where α is a variable parameter [15, 16].

The reduced reciprocal Randić index, that is the reduced analogue of The reciprocal Randić index and is defined as

$$RRR = RRR(G) = \sum_{uv\in E(G)}\sqrt{(d_u(G)-1)(d_v(G)-1)}$$

In this paper we study two types of TiO_2 NTs based on their structural layers in underlying chemical structure: 3-Layered SW TiO_2 NTs and 6-Layered SW TiO_2 NTs. We will compute all of the above mentioned degree-based topological indices for these structures.

2. Randić indices for 3-layered SW TiO_2 NTs

The existance of TiO_2 NTs, in nature is in two forms namely, single-walled titania nanotubes (SW TiO_2 NTs) and multi-walled titania nanotubes (MW TiO_2 NTs). We are considering their chemical graphs because our aim is to work on molecular descriptors. For this reason our choice is ultimately, SW TiO_2 NTs. The three mineral forms of titanium dioxide are anatase, brookite and rutile [17]. The energetically stable anatase surface contains either six (O–Ti–O–O–Ti-O) or three (O–Ti–O) layers [17]. The two-periodic (2D) sheets cut from this anatase surface are used to form the TiO_2 NTs. If p and q are number of titanium atoms in each column and row respectively then the 2-parametric chemical graph of 3-layered SW TiO_2 NTs is denoted as TNT_3 [p,q], which can be viewed in Fig. 2.1.

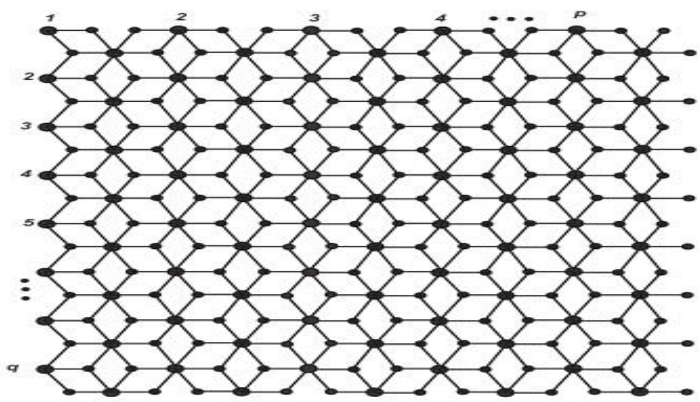

Fig. 2.1. The chemical graph of 3-layered SW TiO_2 NTs

The size of TNT_3 [p,q] is 12pq+2q. There are four kinds of edges corresponding to their degrees of end vertices which are:

$$E_{2,4} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 4 \}$$
$$E_{3,4} = \{ uv \in E(G) \mid d_u(G) = 3 \text{ and } d_v(G) = 4 \}$$
$$E_{2,6} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 6 \}$$
$$E_{3,6} = \{ uv \in E(G) \mid d_u(G) = 3 \text{ and } d_v(G) = 6 \}$$

The edge partition of edge set of the 3-layered SW TiO_2 NTs along with their cardinalities is shown in Table 2.1.

Table 2.1.

Edge partition of edge set of TNT_3 [p,q]

E_{d_u,d_v}	$E_{2,4}$	$E_{3,4}$	$E_{2,6}$	$E_{3,6}$
Cardinality of E_{d_u,d_v}	4p	4p	4p	2p(6q-5)

Now we present the formulae of Randić indices for 3-layered SW TiO_2 NTs by use the edge partitions given in Tabel 2.1.

Theorem 2.1. The general Randić index for 3-layered SW TiO_2 NTs is given by

$$R_\alpha(G) = [2^{\alpha+1} p(2^\alpha + 2.3^\alpha) + 3^{2\alpha}(6q-5)]2^{\alpha+1} p$$

Proof. Since $R_\alpha(G) = \sum_{uv\in E(G)} (d_u(G)d_v(G))^\alpha$

$$= 8^\alpha |E_{2,4}| + (12)^\alpha |E_{3,4}| + (12)^\alpha |E_{2,6}| + (18)^\alpha |E_{3,6}|$$

$$= 4p8^\alpha + 4p(12)^\alpha + 4p(12)^\alpha + 2p(6q-5)(18)^\alpha$$

$$= [2^{\alpha+1}(2^\alpha + 2.3^\alpha) + 3^{2\alpha}(6q-5)]2^{\alpha+1} p$$

Theorem 2.2. The Randić indices for 3-layered SW TiO_2 NTs for $\alpha = \frac{1}{2}, -\frac{1}{2}, 1, -1$ are as under

$$(i).\ R_{\frac{1}{2}}(G) = RR(G) = [8\sqrt{3} + \sqrt{2}(18q-11)]2p$$

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

$$(iii).\ R(G) = 4p(54q-13)$$

$$(iv).\ R_{-1}(G) = \frac{p}{18}(12q+11)$$

Proof. $(i).\ R_{\frac{1}{2}}(G) = RR(G) = \sum_{uv\in E(G)} \sqrt{d_u(G)d_v(G)}$

$$= \sqrt{8}|E_{2,4}| + \sqrt{12}|E_{3,4}| + \sqrt{12}|E_{2,6}| + \sqrt{18}|E_{3,6}|$$

$= 4p\sqrt{8} + 4p\sqrt{12} + 4p\sqrt{12} + 2p(6q-5)\sqrt{18} = [8\sqrt{3} + \sqrt{2}(18q-11)]2p$

$$(ii).\ R_{-\frac{1}{2}}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u(G)d_v(G)}}$$

$$= \frac{1}{\sqrt{8}}|E_{2,4}| + \frac{1}{\sqrt{12}}|E_{3,4}| + \frac{1}{\sqrt{12}}|E_{2,6}| + \frac{1}{\sqrt{18}}|E_{3.6}|$$

$$= \frac{4p}{\sqrt{8}} + \frac{4p}{\sqrt{12}} + \frac{4p}{\sqrt{12}} + \frac{12pq-10p}{\sqrt{18}} = \frac{2\sqrt{2}p}{3}(3q-1+\sqrt{6})$$

$$(iii).\ R(G) = \sum_{uv\in E(G)} d_u(G)d_v(G)$$

$$= 8|E_{2,4}| + 12|E_{3,4}| + 12|E_{2,6}| + 18|E_{3.6}|$$

$$= 4p(8) + 4p(12) + 4p(12) + (12pq-10p)(18) = 4p(54q-13)$$

$$(iv).\ R_{-1}(G) = \sum_{uv\in E(G)} \frac{1}{d_u(G)d_v(G)}$$

$$= \frac{1}{8}|E_{2,4}| + \frac{1}{12}|E_{3,4}| + \frac{1}{12}|E_{2,6}| + \frac{1}{18}|E_{3.6}|$$

$$= \frac{4p}{8} + \frac{4p}{12} + \frac{4p}{12} + \frac{12pq-10p}{18} = \frac{p}{18}(12q+11)$$

For the choice of $\alpha = \frac{1}{2}$, the general Randić index becomes reduced Randić index and for $\alpha = 1$ it reduces to second Zagreb index. Because of this we have tested the general Randić index for $\alpha = \frac{1}{2}, -\frac{1}{2}, 1, -1$.

Theorem 2.3. The reduced reciprocal Randić index for 3-layered SW TiO_2 NTs is given by

$$RRR(G) = 4p(\sqrt{3} + \sqrt{5} + \sqrt{6}) + 2\sqrt{10}p(6q-5)$$

Proof. $RRR(G) = \sum_{uv\in E(G)} \sqrt{(d_u(G)-1)(d_v(G)-1)}$

$$= \sqrt{3}|E_{2,4}| + \sqrt{6}|E_{3,4}| + \sqrt{5}|E_{2,6}| + \sqrt{10}|E_{3,6}|$$

$$= 4p(\sqrt{3}) + 4p(\sqrt{6}) + 4p(\sqrt{5}) + (12pq-10p)(\sqrt{10})$$

$$= 4p(\sqrt{3} + \sqrt{5} + \sqrt{6}) + 2\sqrt{10}p(6q-5)$$

3. Randić indices for 6-layered SW TiO_2 NTs

The graph of 6-layered SW TiO_2 NTs can be viewed as in Fig. 3.1. The 2-parametric chemical graph of 6-layered SW TiO_2 NTs is denoted by TNT_6 [p,q]. It is defined periodically as shown in Fig. 3.1, where p and q are number of titanium atoms in each column and each row respectively.

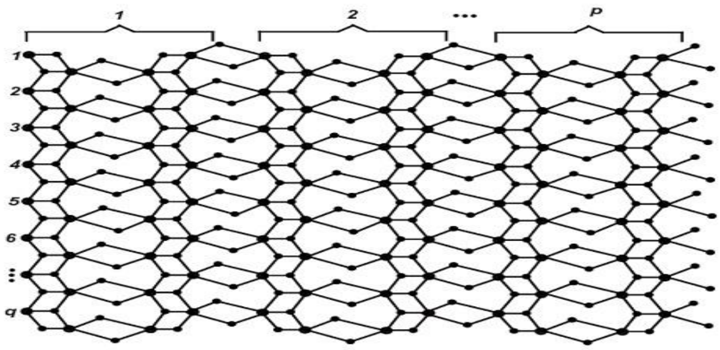

Fig. 3.1. The graph of 6-layered SW TiO_2 NTs

The size of TNT_6 [p,q] is 20pq + 2p. There are six kinds of edges corresponding to their degrees of end vertices which are

$E_{2,2} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 2 \}$
$E_{2,3} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 3 \}$
$E_{2,4} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 4 \}$
$E_{2,5} = \{ uv \in E(G) \mid d_u(G) = 2 \text{ and } d_v(G) = 5 \}$
$E_{3,4} = \{ uv \in E(G) \mid d_u(G) = 3 \text{ and } d_v(G) = 4 \}$
$E_{3,5} = \{ uv \in E(G) \mid d_u(G) = 3 \text{ and } d_v(G) = 5 \}$

The edge partition of edge set of TNT_6 [p,q] along with their cardinalities can be seen in Table 3.1.

Table 3.1.

Edge partition of edge set of TNT_6 [p,q]

E_{d_u,d_v}	$E_{2,2}$	$E_{2,3}$	$E_{2,4}$	$E_{2,5}$	$E_{3,4}$	$E_{3,5}$
Cardinality of E_{d_u,d_v}	2p	2p	6p	8pq	2p	2p(6q-5)

Following theorems exhibit the Randić indices for 6-layered SW TiO_2 NTs.

Theorem 3.1. The general Randić index for 6-layered SW TiO_2 NTs is given by*y*

$$R_\alpha(G) = 2^{\alpha+1} p(2^\alpha + 3^\alpha + 3.4^\alpha + 6^\alpha) + 2p5^\alpha(2.3^{\alpha+1}q + 2^{\alpha+2}q - 5.3^\alpha)$$

Proof. $R_\alpha(G) = \sum_{uv\in E(G)} (d_u(G)d_v(G))^\alpha$

$$= 4^\alpha |E_{2,2}| + 6^\alpha |E_{2,3}| + 8^\alpha |E_{2,4}| + (10)^\alpha |E_{2,5}| + (12)^\alpha |E_{3,4}| + (15)^\alpha |E_{3,5}|$$

$$= 2p4^\alpha + 2p6^\alpha + 6p8^\alpha + 2p(12)^\alpha + 8pq(10)^\alpha + 2p(6q-5)(15)^\alpha$$

$$= 2^{\alpha+1} p(2^\alpha + 3^\alpha + 3.4^\alpha + 6^\alpha) + 2p5^\alpha(2.3^{\alpha+1}q + 2^{\alpha+2}q - 5.3^\alpha)$$

Theorem 3.2. The Randić indices of 6-layered SW TiO_2 NTs for $\alpha = \frac{1}{2}, -\frac{1}{2}, 1, -1$ are as under

$(i).\ R_{\frac{1}{2}}(G) = RR(G) = [2\sqrt{5}q(3\sqrt{3} + 2\sqrt{2}) + 2 + 2\sqrt{3} + \sqrt{6} + 6\sqrt{2} - 5\sqrt{15}]2p$

$(ii).\ R_{-\frac{1}{2}}(G) = \frac{p}{\sqrt{6}}(\sqrt{2} + 2 + \sqrt{6} + 3\sqrt{3} - 2\sqrt{10}) + \frac{4pq}{\sqrt{5}}(\sqrt{2} + \sqrt{3})$

$(iii).\ R(G) = 2p(130q - 29)$

$(iv).\ R_{-1}(G) = \frac{p}{60}(96q + 65)$

Proof. $(i).\ R_{\frac{1}{2}}(G) = RR(G) = \sum_{uv \in E(G)} \sqrt{d_u(G)d_v(G)}$

$= \sqrt{4}|E_{2,2}| + \sqrt{6}|E_{2,3}| + \sqrt{8}|E_{2,4}| + \sqrt{10}|E_{2,5}| + \sqrt{12}|E_{3,4}| + \sqrt{15}|E_{3,5}|$

$= 2p\sqrt{4} + 2p\sqrt{6} + 6p\sqrt{8} + 2p\sqrt{12} + 8pq\sqrt{10} + 2p(6q - 5)\sqrt{15}$

$= [2\sqrt{5}q(3\sqrt{3} + 2\sqrt{2}) + 2 + 2\sqrt{3} + \sqrt{6} + 6\sqrt{2} - 5\sqrt{15}]2p$

$(ii).\ R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u(G)d_v(G)}}$

$= \frac{1}{\sqrt{4}}|E_{2,2}| + \frac{1}{\sqrt{6}}|E_{2,3}| + \frac{1}{\sqrt{8}}|E_{2,4}| + \frac{1}{\sqrt{12}}|E_{3,4}| + \frac{1}{\sqrt{10}}|E_{2,5}| + \frac{1}{\sqrt{15}}|E_{3,5}|$

$= \frac{2p}{\sqrt{4}} + \frac{2p}{\sqrt{6}} + \frac{6p}{\sqrt{8}} + \frac{2p}{\sqrt{12}} + \frac{8pq}{\sqrt{10}} + \frac{12pq - 10p}{\sqrt{15}}$

$= \frac{p}{\sqrt{6}}(\sqrt{2} + 2 + \sqrt{6} + 3\sqrt{3} - 2\sqrt{10}) + \frac{4pq}{\sqrt{5}}(\sqrt{2} + \sqrt{3})$

$(iii).\ R(G) = \sum_{uv \in E(G)} d_u(G)d_v(G)$

$= 4|E_{2,2}| + 6|E_{2,3}| + 8|E_{2,4}| + 12|E_{3,4}| + 10|E_{2,5}| + 15|E_{3,5}|$

$= 2p(4) + 2p(6) + 6p(8) + 2p(12) + 8pq(10) + (12pq - 10p)(15)$

$= 2p(130q - 29)$

$(iv).\ R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{d_u(G)d_v(G)}$

$= \frac{|E_{2,2}|}{4} + \frac{|E_{2,3}|}{6} + \frac{|E_{2,4}|}{8} + \frac{|E_{3,4}|}{12} + \frac{|E_{2,5}|}{10} + \frac{|E_{3,5}|}{15}$

$= \frac{2p}{4} + \frac{2p}{6} + \frac{6p}{8} + \frac{2p}{12} + \frac{8pq}{10} + \frac{12pq - 10p}{15} = \frac{p}{60}(96q + 65)$

Theorem 3.3. The reduced reciprocal Randić index for 6-layered SW TiO_2 NTs is given by

$$RRR(G) = 2p(1-9\sqrt{2}+\sqrt{6}+3\sqrt{3})+8pq(2+3\sqrt{2})$$

Proof. $RRR(G) = \sum_{uv\in E(G)}\sqrt{(d_u(G)-1)(d_v(G)-1)}$

$$=|E_{2,2}|+\sqrt{2}|E_{2,3}|+\sqrt{3}|E_{2,4}|+\sqrt{6}|E_{3,4}|+\sqrt{4}|E_{2,5}|+\sqrt{8}|E_{3,5}|$$

$$= 2p+2p(\sqrt{2})+6p(\sqrt{3})+2p(\sqrt{6})+8pq\sqrt{4}+(12pq-10p)(\sqrt{8})$$

$$= 2p(1-9\sqrt{2}+\sqrt{6}+3\sqrt{3})+8pq(2+3\sqrt{2})$$

4. Conclusion and general remarks

In this paper, we have conducted the study of Randić indices for two types of SW TiO_2 NTs: 3-layered and 6-layered SW TiO_2 NTs. The Randić index was not only much studied by both chemists and mathematicians but was a subject of a variety of modifications and generalizations. We presented the exact formulae of Randić indices for these SW TiO_2 NTs. Various graph-theoretic parameters and certain distance based and counting related topological descriptors for these SW TiO_2 NTs are still open problems.

R E F E R E N C E S

[1] *I. Gutman, O. Polansky*, Springer-Verlag, Berlin. http://dx.doi. org/ 10. 1007/978-3-642-70982-1, (1986).
[2] *N. Trinajstić*, CRC Press, Boca Raton, FL. (1992).
[3] *J. Zhao, X. Wang, T. Sun, L. Li*, Nanotechnology, **16**, 2450 (2005).
[4] *Y. Z. Li, N. H. Lee, E. G. Lee, J. S. Song, S. J. Kim*, Chem. Phys. Lett., **389**, 124(2004).
[5] *D. V. Bavykin, J. M. Friedrich, F. C. Walsh*, F.C., Advanced. Materials, **18**, 2807(2016).
[6] *W. Wang, O. K. Varghese, M. Paulose, C. A. Grimes*, J. Mater. Res., **19**, 417(2004).
[7] *I. Gutman, N. Trinajstić*, Chem.Phy.Lett., **17**, 535(1972).
[8] *I.Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox*, J. Chem. Phys., **62**, 1692(1975).
[9] *A. T. Balaban, I. Motoc, D. Bonchev, O. Makenyan*, Topics Curr. Chem., 114, 21(1983).
[10] *M. Randić*, J. Am. Chem. Soc., **97**, 6609(1975).
[11] *L. B. Kier, L. H. Hall, W. J. Murray, M. Randić*, J. Pharm. Sci., **64**, 1971(1975).
[12] *L. B. Kier, L. H. Hall*, Academies Press, New York, (1976).
[13] *B. Bollobás, P. Erdös*, Ars. Combinatoria, **50**, 225(1998).
[14] *D. Amić, D. Bešlo, B. Lucić, S. Nikolić, N. Trinajstić*, J. Chem. Inf. Comput. Sci., **38**, 819(1998).
[15] *I. Gutman, B. Furtula*, Univ. Kragujevac, Kragujevac, (2008).
[16] *X. Li, I. Gutman*, Univ. Kragujevac, Kragujevac. (2006)
[17] *R. A. Evarestov, A. V. Bandura, M. V. Losev, S. Piskunov, Yu. F. Zhukovskii*, Physica E., **43**, 266(2010).