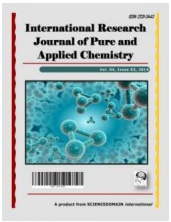

International Research Journal of Pure & Applied Chemistry

16(4): 1-9, 2018; Article no.IRJPAC.42645
ISSN: 2231-3443, NLM ID: 101647669

M-Polynomial and Degree Based Topological Indices for Silicon Oxide

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Authors' contributions

This work was carried out in collaboration between all authors. Authors PJNT and PE designed the study, wrote the protocol and wrote the first draft of the manuscript. Author MK designed the Chemistry part of the paper and wrote the description of the Silicon oxide. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/IRJPAC/2018/42645
Editor(s):
(1) Dr. Wolfgang Linert, Professor, Institute of Applied Synthetic Chemistry, Vienna University of Technology Getreidemarkt, Austria.
Reviewers:
(1) Rachanna Kanabur, BLDE Association's Commerce, BHS Arts & TGP Science College, India.
(2) Nazeer Muhammad, COMSATS Institute of Information Technology, Pakistan.
(3) Donald H. Galvan, Universidad Nacional Autonoma de Mexico.
(4) Fatma Kandemirli, Kastamonu University, Turkey.
Complete Peer review History: http://www.sciencedomain.org/review-history/25449

Original Research Article

Received 26th April 2018
Accepted 30th June 2018
Published 7th July 2018

ABSTRACT

Silican oxide (SiO_2) is the most abundant oxide present on the surface of the earth which has a wide spectrum of technological applications due to it's various chemical and physical properties. The topological index is a numerical representation of a molecular structure. The first topological index in chemical graph theory is the Winer index which is a distance-based topological index. The degree-based topological indices are the most studied type of topological indices which play a prominent role in chemical graph theory. In this paper, we derive the *M*-Polynomial for Silican oxide SiO_2 layer structure and calculate some of the important degree based topological indices using this *M*-polynomial. We derive the *M*-Polynomial derivative formula for the *ABC*-index and calculate the *ABC*-index by using this derived formula.

Keywords: M-polynomials; chemical graph theory; silicon oxide; topological index.

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1. INTRODUCTION

Silica (SiO_2) is the most abundant oxide present on the surface of the earth [1]. Silicon forms compound with oxygen called silicates and the basic unit of silicate is a tetrahedral ion, $[SiO_4]^{4-}$ which linking to self-similar units sharing one, two, three, or all four corner oxygens of the tetrahedron. Silica gives a variety of physical properties such as surface stress, density, refractive index, and temperature due to its different crystalline polymorphs [2]. These polymorphs have identical chemical composition. However, the atomic arrangements are different from each other. Most of the silica polymorphs, Si forms tetrahedral coordination with oxygen whereas in some conditions, it form the octahedral coordination with oxygen [2]. SiO_2 has a wide spectrum of technological applications due to its various chemical and physical properties [3]. Fig. 1 shows that the Silicate which consists of a Si and four oxygen and this tetrahedron structure having a four-negative charge.

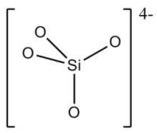

Fig.1. Silicate

This tetrahedral structure is linked at the corners by oxygen-to-oxygen covalent bonds and form the network structure as shown in Fig. 2 and 3 [4]. This silicate forms the network structure when it polymerizes as shown in Fig. 2 and 3.

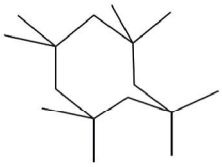

Fig. 2. SiO_2 Network [4]

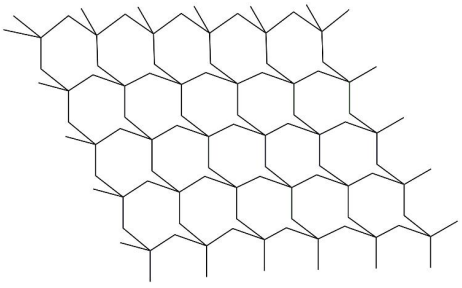

Fig. 3. SiO_2 Network Structure [4]

The topological index is a numerical representation of a molecular structure. In molecular graphs, the atoms and the chemical bonds between them are represented by vertices and edges respectively in the graph theory. A graph $G = G(V, E)$ is a pair $V = V(G)$ of nonempty set of vertices and $E = E(G)$ of the set of connected edges if there exists a connection between any pair of vertices in G. For a connected graph G and vertices u, v in the set of vertices $V(G)$, the degree is the number of vertices which are connected to that vertex by the edges and is denoted by $d_v(G)$ or d_v. It is noted that the degree of any vertex in a chemical graph is at most four. The concept of degree is closely related to the concept of valence bond in chemistry. The distance between two vertices u and v is the length of the shortest path between these vertices and is denoted by $d(u, v)$ or $d_G(u, v)$. The first and the most studied topological index in chemical graph theory is the Winer index which was introduced by the chemist H. Wiener [5] in 1947. This is a distance-based topological index which was used to demonstrate correlations between physicochemical properties of organic compounds and the topological structure of their molecular graphs by Wiener. The degree-based topological indices are the most studied type of topological indices which play a prominent role in chemical graph theory. One of the oldest degree-based topological indices is the Zagreb index which was introduced by Gutman and Trinajstic [6] during the analysis of the structure-dependency of total-electron energy. The first Zagreb index $M_1(G)$ was defined as

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 = \sum_{uv \in E(G)} (d_u + d_v)$$

and the second Zagreb index $M_2(G)$ was defined as

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

The second modified Zagreb index which was introduced by Hao [7] was defined as

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

The Randić index which is also one of the oldest topological indices was introduced by Randić [8]. This was defined as

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

The Randić index is one of the most studied, most often applied and most popular degree-based topological index in the field of drug design. This index was globalized and recognized as the generalized Randić index and defined as

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

where α is an arbitrary real number [9]. When $\alpha = -\frac{1}{2}$, the above generalized Randić index becomes the (original) Randić index. The following formula is also called the generalized Randić index [10] and defined as

$$RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}.$$

The atom-based connectivity index abbreviated by *ABC*-index was introduced by Ernesto Estrada [11]. This is an amended version of the Randić index and is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The *ABC*-index has excellent correlation with the thermodynamic properties of alkanes, especially with their heats of formation. Furtula et al. [12] introduced the augmented Zagreb index which was useful for computing heat formation of alkanes and defined as

$$AZI(G) = \sum_{uv \in E(G)} \left\{\frac{d_u d_v}{d_u + d_v - 2}\right\}^3.$$

The *ABC*-index can be derived from this augmented Zagreb index by replacing its power 3 by the power -0.5.

The harmonic index was first introduced by Siemion Fajtlowicz [13] and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

This is actually another variant of the Randić index. Favaron et al. [14] showed the relation between the harmonic index and the eigen values of graphs. A significant predictor of the total surface area of octane isomers is the inverse sum index [15] which was defined as

$$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

The symmetric division index is used to characterize the chemical and physical properties of molecules and defined as

$$SDD(G) = \sum_{uv \in E(G)} \left\{\frac{\min(d_u, d_{v)}}{\max(d_u, d_{v)}} + \frac{\max(d_u, d_{v)}}{\min(d_u, d_{v)}}\right\}.$$

The forgotten topological index is another degree-based topological index in which some recent researches were conducted. The forgotten topological index for some dendrimers structure was discussed in [16]. Some recent researches on the reciprocal Randic*'* index, the reduced second Zagreb index, and the reduced reciprocal Randic*'* index of Poly (Propyl) Ether Imine, porphyrin and Zinc-Porphyrin dendrimers were discussed in [17].

Algebraic polynomials play an important role to study the structural properties of the molecules in mathematical chemistry. The Hosoya polynomial (also known as the Wiener polynomial) was used for the determination of the distance-based topological indices. For the study of the degree-based topological indices, the *M*-polynomial which is another important polynomials in the study of the structural properties of molecules were used. This is introduced by Deutsch and Klavzar [10] in 2015.

Theorem 1 [10]

Let $G = G(V, E)$ be a graph and let $m_{ij}(G), i, j \geq 1$, be the number of edges $e = uv$ of G such that $\{d_v, d_u\} = \{i, j\}, u, v \in V(G)$. Then the *M*-polynomial of G is

$$M(G; x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j$$

.

Some of the degree-based topological indices were derived from *M*-polynomial and given in the Table 1.

Table 1. Some standard degree-based topological indices and the derived formulas to compute them from the *M*-polynomial [10]

Topological index	$f(x, y)$	Derivation from $M(G; x, y)$
General Randić ($\alpha \in \mathbb{N}$)	$(xy)^{\alpha}$	$\left(D_x^{\alpha} D_y^{\alpha}\right)\left(M(G; x, y)\right)_{x=y=1}$
General Randić ($\alpha \in \mathbb{N}$)	$\frac{1}{(xy)^{\alpha}}$	$\left(S_x^{\alpha} S_y^{\alpha}\right)\left(M(G; x, y)\right)_{x=y=1}$
First Zagreb	$x + y$	$\left(D_x + D_y\right)\left(M(G; x, y)\right)_{x=y=1}$
Second Zagreb	xy	$\left(D_x D_y\right)\left(M(G; x, y)\right)_{x=y=1}$
Second modified Zagreb	$\frac{1}{xy}$	$\left(S_x S_y\right)\left(M(G; x, y)\right)_{x=y=1}$
Augmented Zagreb index	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 \left(M(G; x, y)\right)_{x=y=1}$
Harmonic index	$\frac{2}{x+y}$	$2 S_x J \left(M(G; x, y)\right)_{x=1}$
Inverse sum index	$\frac{xy}{x+y}$	$S_x J D_x D_y \left(M(G; x, y)\right)_{x=1}$
Symmetric division index	$\frac{x^2+y^2}{xy}$	$\left(D_x S_y + S_x D_y\right)\left(M(G; x, y)\right)_{x=y=1}$

where ,

$D_x = x \frac{\partial f(x,y)}{\partial x}$, $D_y = y \frac{\partial f(x,y)}{\partial y}$

$S_x = \int_0^x \frac{f(t,y)}{t} dt$, $S_y = \int_0^y \frac{f(x,t)}{t} dt$,

$J\left(f(x,y)\right) = f(x,x)$ and $Q_{\alpha}\left(f(x,y)\right) = x^{\alpha} f(x,y)$.

2. MATERIALS AND METHODS

The degree based topological indices by using *M*-polynomial are calculated for the (p, q) - layer structure of SiO_2 for arbitrary values of p and q, where p is the number of rows and q is the number of Silicate in a row. We have seen in Figure 3 that there are two types of edge partition for the structure of SiO_2 layer which are (1,4) type with the end vertices of the edge are of degrees 1 and 4 and (2,4) type the end vertices of the edge are of degrees 2 and 4. The details of these are summarized in Table 2.

Table 2. The edge partition of SiO_2 layer

Edge partition (d_u, d_v)	$(1, 4)$	$(2, 4)$
Number of edges	$2p + 2q + 4$	$2p + 2q + 4pq$

Theorem 2

Let $G = SiO_2$ be the silicon layer structure. Then the *M*-polynomial for the silicon layer structure is given by

$$M(SiO_2; x, y) = (2p + 2q + 4)xy^4 + (2p + 2q + 4pq)x^2y^4.$$

Proof.

The silicon layer structure SiO_2 is given in the figure 3. Using the edge partition given in the Table 2, we get the *M*-polynomial of SiO_2as

$$\begin{aligned} M(SiO_2; x, y) &= \sum_{i \le j} m_{ij} x^i y^j \\ &= m_{14}x^1y^4 + m_{24}x^2y^4 \\ &= (2p + 2q + 4)xy^4 + (2p + 2q + 4pq)x^2y^4 \end{aligned}$$

Theorem 3

Let $G = SiO_2$ be the silicon layer structure, then the degree-based topological indices for SiO_2 are

1. $M_1(SiO_2) = 22(p + q) + 24pq + 20$
2. $M_2(SiO_2) = 24(p + q) + 32pq + 16.$
3. ${}^{m}M_2(SiO_2) = \frac{3}{4}(p + q) + \frac{1}{2}pq + 1.$
4. $RR_\alpha(SiO_2) = (2^{2\alpha+1} + 2^{3\alpha+1})(p + q) + 2^{3\alpha+1}pq + 2^{2\alpha+1}$
5. $SDD(SiO_2) = \frac{27}{2}(p + q) + 10pq + 17.$

Proof. Let $f(x, y)$ be the M-polynomial of SiO_2. Then

$$f(x, y) = M(SiO_2; x, y) = (2p + 2q + 4)xy^4 + (2p + 2q + 4pq)x^2y^4$$

and we get the following

$$D_x\big(f(x, y)\big) = (2p + 2q + 4)xy^4 + 2(2p + 2q + 4pq)x^2y^4,$$

$$D_y\big(f(x, y)\big) = 4(2p + 2q + 4)xy^4 + 4(2p + 2q + 4pq)x^2y^4,$$

$$D_xD_y\big(f(x, y)\big) = 4(2p + 2q + 4)xy^4 + 8(2p + 2q + 4pq)x^2y^4,$$

$$S_x(f(x, y)) = (2p + 2q + 4)xy^4 + (p + q + 2pq)x^2y^4,$$

$$S_y(f(x, y)) = \frac{1}{2}(p + q + 2)xy^4 + \frac{1}{2}(p + q + 2pq)x^2y^4,$$

$$S_xS_y\big(f(x, y)\big) = \frac{1}{2}(p + q + 2)xy^4 + \frac{1}{4}(p + q + 2pq)x^2y^4,$$

$$D_y^\alpha\big(f(x, y)\big) = 4^\alpha(2p + 2q + 4)xy^4 + 4^\alpha(2p + 2q + 4pq)x^2y^4$$

$$D_x^\alpha D_y^\alpha\big(f(x, y)\big) = 4^\alpha(2p + 2q + 4)xy^4 + 2^\alpha.4^\alpha(2p + 2q + 4pq)x^2y^4,$$

$$S_y^{\alpha}(f(x,y)) = \frac{(2p+2q+4)}{4^{\alpha}}xy^4 + \frac{(2p+2q+4pq)}{4^{\alpha}}x^2y^4,$$

$$S_x^{\alpha}S_y^{\alpha}(f(x,y)) = \frac{(2p+2q+4)}{4^{\alpha}}xy^4 + \frac{(2p+2q+4pq)}{2^{\alpha}.4^{\alpha}}x^2y^4,$$

$$D_xS_y(f(x,y)) = \frac{1}{2}(p+q+2)xy^4 + (p+q+2pq)x^2y^4,$$

$$S_xD_y(f(x,y)) = 4(2p+2q+4)xy^4 + 2(2p+2q+4pq)x^2y^4.$$

Using the derived formulas of M-polynomial given in the table 1, we find

1. $M_1(SiO_2) = \big(D_x + D_y\big)\big(f(x,y)\big)|_{x=y=1} = 22(p+q) + 24pq + 20.$
2. $M_2(SiO_2) = D_xD_y\big(f(x,y)\big)|_{x=y=1} = 24(p+q) + 32pq + 16.$
3. $^{m}M_2(SiO_2) = S_xS_y\big(f(x,y)\big)|_{x=y=1} = \frac{3}{4}(p+q) + \frac{1}{2}pq + 1.$
4. $R_{\alpha}(SiO_2) = D_x^{\alpha}D_y^{\alpha}\big(f(x,y)\big)|_{x=y=1} = \left(\frac{2}{4^{\alpha}} + \frac{2}{8^{\alpha}}\right)(p+q) + \frac{4}{8^{\alpha}}pq + \frac{4}{4^{\alpha}}.$
5. $RR_{\alpha}(SiO_2) = S_x^{\alpha}S_y^{\alpha}(f(x,y))|_{x=y=1} = (2^{2\alpha+1} + 2^{3\alpha+1})(p+q) + 2^{3\alpha+1}pq + 2^{2\alpha+1}.$
6. $SDD(SiO_2) = (D_xS_y + S_xD_y)(f(x,y))|_{x=y=1} = \frac{27}{2}(p+q) + 10pq + 17.$

Theorem 4. Let $G = SiO_2$ be the silicon layer structure, then

1. $H(SiO_2) = \frac{22}{15}(p+q) + \frac{4}{3}pq + \frac{8}{5}.$
2. $I(SiO_2) = \frac{64}{15}(p+q) + \frac{16}{3}pq + \frac{16}{5}.$
3. $AZI(SiO_2) = \frac{560}{27}(p+q) + 32pq + \frac{256}{27}.$

Proof: The *M*-polynomial of SiO_2 is

$$f(x,y) = (2p+2q+4)xy^4 + (2p+2q+4pq)x^2y^4$$

and we get the following

$$J\big(f(x,y)\big) = (2p+2q+4)x^5 + (2p+2q+4pq)x^6,$$

$$S_xJ\big(f(x,y)\big) = \frac{(2p+2q+4)}{5}x^5 + \frac{(2p+2q+4pq)}{3}x^6,$$

$$JD_xD_y\big(f(x,y)\big) = 4(2p+2q+4)x^5 + 8(2p+2q+4pq)x^6,$$

$$S_xJD_xD_y\big(f(x,y)\big) = \frac{4}{5}(2p+2q+4)x^5 + \frac{8}{6}(2p+2q+4pq)x^6,$$

$$D_y^3\big(f(x,y)\big) = 4^3(2p+2q+4)xy^4 + 4^3(2p+2q+4pq)x^2y^4,$$

$$D_x^3D_y^3\big(f(x,y)\big) = 4^3(2p+2q+4)xy^4 + 2^3.4^3(2p+2q+4pq)x^2y^4,$$

$$JD_x^3D_y^3\big(f(x,y)\big) = 4^3(2p+2q+4)x^5 + 2^3.4^3(2p+2q+4pq)x^6,$$

$$Q_{-2}JD_x^3D_y^3\big(f(x,y)\big) = 4^3(2p+2q+4)x^3 + 2^3.4^3(2p+2q+4pq)x^4,$$

$$S_x^3Q_{-2}JD_x^3D_y^3\big(f(x,y)\big) = \frac{4^3(2p+2q+4)}{3^3}x^3 + \frac{2^3.4^3}{4^3}(2p+2q+4pq)x^4.$$

Again using the derived formulas of *M*-polynomial given in the table 1, we find

1. $H(SiO_2) = 2S_xJ\big(f(x,y)\big)|_{x=y=1} = \frac{22}{15}(p+q) + \frac{4}{3}pq + \frac{8}{5}$
2. $I(SiO_2) = S_xJD_xD_y(f(x,y))|_{x=y=1} = \frac{64}{15}(p+q) + \frac{16}{3}pq + \frac{16}{5}$..
3. $AZI(SiO_2) = S_x^3Q_{-2}JD_x^3D_y^3\big(f(x,y)\big)|_{x=y=1} = \frac{560}{27}(p+q) + 32pq + \frac{256}{27}$.

We now propose the derivative formula for the *M*-polynomial of the Atom-Bond connectivity index and illustrate the proof by calculating the ABC-index by using this proposed formula and by direct calculation.

Theorem 5

The *M*-polynomial derivative formula of the Atom-Bond Connectivity index for

SiO_2, is given by the formula

$$ABC(SiO_2) = S_x^{-1/2}Q_{-2}JD_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big)|_{x=y=1}$$

Proof. Using the definition of the Atom-Bond Connectivity (ABC) index, we calculate the ABC index for the SiO_2 layer structure as

$$\begin{aligned} ABC(SiO_2) &= \sum_{UV\epsilon e(SiO_2)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}} \\ &= (2p+2q+4)\sum_{UV\epsilon e(SiO_2)}\sqrt{\frac{1+4-2}{4}} \\ &\quad + (2p+2q+4pq)\sum_{UV\epsilon e(SiO_2)}\sqrt{\frac{2+4-2}{8}} \\ &= \big(\sqrt{2}+\sqrt{3}\big)(p+q) + 2\sqrt{2}pq + 2\sqrt{3}). \end{aligned}$$

Now using the Theorem 5, we again calculate the ABC index of the SiO_2 layer structure as

$$D_y^{-1/2}\big(f(x,y)\big) = 4^{-1/2}(2p+2q+4)xy^4 + 4^{-1/2}(2p+2q+4pq)x^2y^4,$$

$$D_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big) = 4^{-1/2}(2p+2q+4)xy^4 + 2^{-1/2}\times 4^{-1/2}(2p+2q+4pq)x^2y^4,$$

$$JD_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big) = 4^{-1/2}(2p+2q+4)x^5 + 2^{-1/2}\times 4^{-1/2}(2p+2q+4pq)x^6,$$

$$Q_{-2}JD_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big) = 4^{-1/2}(2p+2q+4)x^3 + 2^{-1/2}\times 4^{-1/2}(2p+2q+4pq)x^4,$$

$$S_x^{-1/2}Q_{-2}JD_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big) = \frac{4^{-1/2}(2p+2q+4)}{3^{-1/2}}x^3 + \frac{2^{-1/2}\times 4^{-1/2}}{4^{-1/2}}(2p+2q+4pq)x^4.$$

Therefore, the ABC index for the layer SiO_2 structure is

$$\begin{aligned} ABC(SiO_2) &= S_x^{-1/2}Q_{-2}JD_x^{-1/2}D_y^{-1/2}\big(f(x,y)\big)|_{x=y=1} \\ &= \big(\sqrt{2}+\sqrt{3}\big)(p+q) + 2\sqrt{2}pq + 2\sqrt{3}). \end{aligned}$$

This shows that the *M*- polynomial derivative formula of the Atom-Bond Connectivity index for SiO_2 is the one given in Theorem 5.

3. CONCLUSION

In this paper, we derived the M-Polynomial for Silicon Oxide SiO_2 layer structure and calculated some important degree based topological indices using this *M*-polynomial. We also derived the derived formula of the *M*-polynomial for the *ABC*-index.

ACKNOWLEDGEMENTS

We acknowledge the reviewers for their valuable comments for the improvement of this paper.

COMPETING INTERESTS

The authors declare that there is no conflict of interest regarding the publication of this paper.

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Peer-review history:
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