On Degree-Based Topological Descriptors of Oxide and Silicate Molecular Structures

Haidar Ali [1], Hafiz Muhammad Afzal Siddiqui[2] and Muhammad Kashif Shafiq[1]

[1]Department of Mathematics,
Government College University,
Faisalabad-Pakistan.
[2]Department Of Mathematics,
COMSATS Institute of Information Technology,
Lahore, Pakistan.

Abstract: In this Paper, we study general Zagreb, Zagreb inequality, augmented Zagreb, logarithm of first, second and modified first multiplicative Zagreb indices for Chain Oxide, COX_n, Chain Silicate, CS_n, Sheet Oxide, OX_n and Sheet Silicate, SL_n molecular structures for the first time. Moreover, analytically closed formulae for these structures are determined.

Keywords: Zagreb index, Chain Oxide, Chain Silicate, Sheet Oxide, Sheet Silicate

1. Introduction

A graph $G(V,E)$ with vertex set V and edge set E is connected, if there exist a connection between any pair of vertices in G. A *network* is simply a connected graph having no multiple edges and loops. A *chemical graph* is a graph whose vertices denote atoms and edges denote bonds between the atoms of any underlying chemical structure. The *degree* of a vertex is the number of vertices which are adjacent to that fixed vertex by the edges. In a chemical graph the degree of any vertex is atmost 4. The *distance* between two vertices u and v is denoted as $d(u,v) = d_G(u,v)$ and is the length of shortest path between u and v in graph G. The length of shortest path between u and v is also called $u-v$ *geodesic*. The longest path between any two vertices is called $u-v$ detour.

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity relationships (QSAR) and Quantitative structure-property relationships (QSPR) that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index and ABC index are used to predict bioactivity of the chemical compounds.

A *topological index* is a function "Top" from '$\sum$' to the set of real numbers, where '$\sum$' is the set of finite simple graphs with property that $Top(G) = Top(H)$ if both G and H are isomorphic. There is a lot of research which has been done on topological indices of different graph families so far, and is of much importance due to their chemical significance. A topological index is actually a numeric quantity associated with chemical constitution purporting for correlation of chemical structure with many physico-chemical properties, chemical reactivity or you can say that biological activity. Actually topological indices are designed on the ground of transformation of a molecular graph into a number which characterize the topology of that graph.

In this article, G is considered to be a network with vertex set $V(G)$ and edge set $E(G)$, d_u is the degree of vertex $u \in V(G)$ and $S_u = \sum_{v \in N_G(u)} d(v)$ where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. The notations used in this article are mainly taken from books [7, 9].

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin. He named this index as *path number*. Later on, path number was renamed as *Wiener* index [18] and then theory of topological index started.

Let G be a graph. Then the Wiener index of G is defined as

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u,v)$$

where (u,v) is any ordered pair of vertices in G and $d(u,v)$ is $u-v$ geodesic. The very first and oldest degree based topological index is *Randić* index [17] denoted by $R_{-\frac{1}{2}}(G)$ and introduced by Milan Randić in 1975. The general Randić index was proposed by Bollobás and Erdös [5] and Amic et al. [1] independently, in 1998 . Then it has been extensively studied by both mathematicians and theoretical chemists [13]. Many important mathematical properties have been established [6]. For a survey of results, we refer to the new book by Li and Gutman [16].

The general Randić index $R_\alpha(G)$ is the sum of $(d_u d_v)^\alpha$ over all edges $e = uv \in E(G)$ defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha \qquad (2)$$

Ivan Gutman and Trinajstić is the *Zagreb* index or more precisely first Zagreb index denoted by $M_1(G)$. Consider a graph G, then first Zagreb index is defined as

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v) \qquad (3)$$

The second Zagreb index is defined in the following way. Consider a graph G, then second Zagreb index is defined as

$$M_2(G) = \sum_{uv\in E(G)} (d_u \times d_v) \qquad (4)$$

Pierre Hansen noticed that for numerous graphs with *n* vertices and *m* edges, the Zagreb index inequality satisfied. He conjectured that the inequality holds for all graphs. Damir Vukičević soon found counter examples for this inequality, showing that in the general case Hansen's conjecture was false, but inequality holds for all molecular graphs [10]. Unexpectedly, research along these lines did not stop. For any graph G, the Zagreb index inequality defined as

$$mM_1(G) \le nM_2(G) \qquad (5)$$

Furtula *et al*. [8] put forward its modified version, that they somewhat inadequately named *augmented Zagreb index*. For any graph G, the augmented Zagreb index is defined as

$$AZI(G) = \sum_{u,v} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \qquad (6)$$

For any graph G, the logarithm of first multiplicative Zagreb index is defined as

$$\ln \Pi_1(G) = 2\sum_{u,v} \left(\frac{\ln d_u}{d_u} + \frac{\ln d_v}{d_v}\right) \qquad (7)$$

For any graph G, the logarithm of the modified first multiplicative Zagreb index is defined

$$\ln \Pi_2(G) = \sum_{u,v} \ln(d_u + d_v) \qquad (8)$$

For any graph G, the logarithm of second multiplicative Zagreb index is defined as

$$\ln \Pi_1^*(G) = \sum_{u,v} \ln d_u + \ln d_v \qquad (9)$$

The general first Zagreb index is the first group Zagreb index for any graph G.

The general second Zagreb index is the second group Zagreb index for any graph G.

2 Main results and discussion

The aim of this section, at first, is to compute some topological indices of the molecular graph of chain oxide COX_n as depicted in Fig1a. Hayat et al. studied various degree based topological indices for various structures in [11]. For further study of topological indices of various graph families see [2, 3, 4, 12, 14, 15, 19].

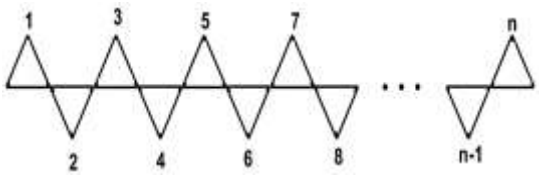

Fig1a: The molecular graph of Chain oxide (COX_n)

Remark 2.1. It is easy to see that $G_1 = COX_n$ has $2n+1$ vertices and $3n$ edges. We partition the edges of G_1 into three subsets $E_1(G_1)$, $E_2(G_1)$ and $E_3(G_1)$. Table 1 shows the number of three types of edges.

From Table 1, we give an explicit computing formula for some indices of Chain oxide shown in Figure 1a.

Theorem 2.1. Consider the graph G_1 of Chain Oxide COX_n. Then

$$(i) M_1(G_1) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$= |E_1|(2+2) + |E_2|(2+4) + |E_3|(4+4)$$
$$= 2(2+2) + 2n(2+4) + (n-2)(4+4)$$
$$= 20n - 8.$$

$$(ii) M_2(G_1) = \sum_{uv \in E(G)} (d_u \times d_v)$$

$$= |E_1|(2\times 2) + |E_2|(2\times 4) + |E_3|(4\times 4)$$
$$= 2(2\times 2) + 2n(2\times 4) + (n-2)(4\times 4)$$
$$= 32n - 24.$$

(d_u, d_v) where $uv \in E(G_1)$	$E_1 = [2,2]$	$E_2 = [2,4]$	$E_3 = [4,4]$
Number of edges	2	$2n$	$n-2$

Table 1: The number of three types of edges of the graph G_1.

$$(iii) mM_1(G_1) \le nM_2(G_1)$$

$$(3n)(20n-8) \le (2n+1)(32n-24), \text{ for } n \ge 2$$

.

$$(iv) AZI(G_1) = \sum_{u,v} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

$$= |E_1|\left(\frac{4}{2}\right)^3 + |E_2|\left(\frac{8}{4}\right)^3 + |E_3|\left(\frac{16}{6}\right)^3$$

$$= 2\left(\frac{4}{2}\right)^3 + 2n\left(\frac{8}{4}\right)^3 + (n-2)\left(\frac{16}{6}\right)^3$$
$$= \frac{944}{27}n + \frac{1456}{27}.$$

$$(v) \ln \Pi_1(G_1) = 2\sum_{u,v} \left(\frac{\ln d_u}{d_u} + \frac{\ln d_v}{d_v}\right)$$

$$= |E_1|\left(2\frac{\ln 2}{2} + 2\frac{\ln 2}{2}\right) + |E_2|\left(2\frac{\ln 2}{4} + 2\frac{\ln 4}{4}\right) +$$
$$|E_3|\left(2\frac{\ln 4}{4} + 2\frac{\ln 4}{4}\right)$$
$$= 2\left(2\frac{\ln 2}{2} + 2\frac{\ln 2}{2}\right) + (2n)\left(2\frac{\ln 2}{4} + 2\frac{\ln 4}{4}\right) +$$
$$(n-2)\left(2\frac{\ln 4}{4} + 2\frac{\ln 4}{4}\right)$$
$$= 2.7724n - 1.3862.$$

$$(vi)\ln \Pi_2(G_1) = \sum_{u,v} \ln(d_u + d_v)$$

$$= |E_1| \ln(2+2) + |E_2| \ln(2+4) + |E_3| \ln(4+4)$$

$$= 2\ln(2+2) + (2n)\ln(2+4) + (n-2)\ln(4+4)$$
$$= 5.6629n - 2.7721.$$

$$(vii)\ln \Pi_1^*(G_1) = \sum_{u,v} \ln d_u + \ln d_v$$

$$= |E_1(\ln 2 + \ln 2) + |E_2(\ln 2 + \ln 4) +$$
$$|E_3(\ln 4 + \ln 4)$$

$$= 2(\ln 2 + \ln 2) + (2n)(\ln 2 + \ln 4) +$$
$$(n-2)(\ln 4 + \ln 4)$$
$$= 6.9314n - 2.7728.$$

Now we present the results for Chain Silicate Network shown in the following figure.

Remark 2.2. We now consider the molecular graph $G_2 = CS_n$, Fig2a. It is easy to see that $|V(G_2)| = 3n+1$ and $|E(G_2)| = 6n$. We partition the edges of G_2 into three subsets $E_1(G_2)$, $E_2(G_2)$ and $E_3(G_3)$. Table 2 shows the number of three types of edges.

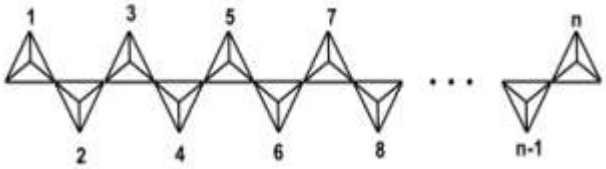

Fig2a: Chain Silicate Network for dimension n.

Theorem 2.2. Consider the graph G_2 of Chain Silicate CS_n. Then

$$(i)M_1(G_2) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$= |E_1|(3+3) + |E_2|(3+6) + |E_3|(6+6)$$

$$= (n+4)(3+3) + (2(2n-1))(3+6) + (n-2)(6+6)$$

$$= 54n - 18.$$

$$(ii)M_2(G_2) = \sum_{uv \in E(G)} (d_u \times d_v)$$

$$= |E_1|(3\times 3) + |E_2|(3\times 6) + |E_3|(6\times 6)$$

$$= (n+4)(3\times 3) + (2(2n-1))(3\times 6) + (n-2)(6\times 6)$$

$$= 117n - 72.$$

$$(iii)mM_1(G_2) \le nM_2(G_2)$$

$$(6n)(54n-18) \le (3n+1)(117n-72), \text{ for } n \ge 2$$

.

$$(iv)AZI(G_2) = \sum_{u,v} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

$$= |E_1|\left(\frac{9}{4}\right)^3 + |E_2|\left(\frac{18}{7}\right)^3 + |E_3|\left(\frac{36}{10}\right)^3$$

Table 2: Edge partition of Chain Silicate Network CS_n based on degrees of end vertices of each edge

.

(d_u, d_v) where $uv \in E(G_2)$	$E_1 = [3,3]$	$E_2 = [3,6]$	$E_3 = [6,6]$
Number of edges	$n+4$	$2(2n-1)$	$n-2$

$$= (n+4)(\frac{9}{4})^3 + (2(2n-1))(\frac{18}{7})^3 + (n-2)(\frac{36}{10})^3$$

$$= (\frac{23328}{343} + \frac{5832}{125} + \frac{729}{64})n + \frac{729}{16} - \frac{11664}{343} - \frac{11664}{125}.$$

$$(vii)\ln \Pi_1^*(G_2) = \sum_{u,v} \ln d_u + \ln d_v.$$

$$=| E_1(\ln 3+\ln 3)+| E_2(\ln 3+\ln 6)+| E_3(\ln 6+\ln 6)$$

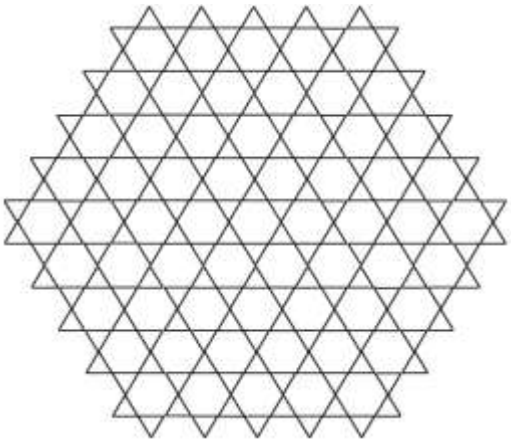

Fig3a: Sheet Oxide Network (OX_5)

$$= (n-4)(\ln 2+\ln 2)+(2(2n-1))(\ln 2+\ln 4)+(n-2)(\ln 4+\ln 4)$$

$$= 17.3423n - 4.1590.$$

$$(v)\ln \Pi_1(G_2) = 2\sum_{u,v}(\frac{\ln d_u}{d_u} + \frac{\ln d_v}{d_v})$$

$$=| E_1 |(2\frac{\ln 3}{3}+2\frac{\ln 3}{3})+| E_2 |(2\frac{\ln 3}{6}+2\frac{\ln 3}{6})+ | E_3 |(2\frac{\ln 6}{6}+2\frac{\ln 6}{6})$$

$$= (n-4)(2\frac{\ln 3}{3}+2\frac{\ln 3}{3})+(2(2n-1))(2\frac{\ln 3}{6}+ 2\frac{\ln 3}{6})+(n-2)(2\frac{\ln 6}{6}+2\frac{\ln 6}{6})$$

$$= 7.9782n - 0.8106.$$

$$(vi)\ln \Pi_2(G_2) = \sum_{u,v} \ln(d_u + d_v)$$

$$=| E_1 |\ln(3+3)+| E_2 |\ln(3+6)+| E_3 |\ln(6+6)$$

$$= (n-4)\ln(3+3)+(2(2n-1))\ln(3+6)+ (n-2)\ln(6+6)$$

$$= 13.0655n - 2.1970$$

Now we present the results for Sheet Oxide Network shown in the following figure.

Remark 2.3. We now consider the molecular graph $G_3 = OX_n$, Figure 3. It is easy to see that $|V(G_3)| = 9n^2 + 3n$ and $|E(G_3)| = 18n^2$. We partition the edges of G_3 into three subsets $E_1(G_3)$ and $E_2(G_3)$. Table 3 shows the number of two types of edges.

Table 3: Edge partition of Sheet Oxide Network OX_n based on degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(G)$	$E_1 = [2,4]$	$E_2 = [4,4]$
Number of edges	$12n$	$18n^2 - 12n$

Theorem 2.3. Consider the graph G_3 of Chain Silicate CS_n. Then

$$(i)M_1(G_3) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$=| E_1 |(2+4)+| E_2 |(4+4)$$

$$= 12n(2+4)+(18n^2 - 12n)(4+4)$$

$$= 24n(6n-1).$$

$$(ii)M_2(G_3) = \sum_{uv \in E(G)} (d_u \times d_v)$$

$=|E_1|(2\times 4)+|E_2|(4\times 4)$

$=12n(2\times 4)+(18n^2-12n)(4\times 4)$
$=96n(3n-1)$.

$$(iii)\, mM_1(G_3)\le nM_2(G_3)$$
$(18n^2)(24n(6n-1))\le(9n^2+3n)(96n(3n-1)),$
$for \quad n\ge 2$

$$(iv)\, AZI(G_3)=\sum_{u,v}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3$$

$=|E_1|(\frac{8}{4})^3+|E_2|(\frac{16}{6})^3$

$=12n(\frac{9}{4})^3+(18n^2-12n)(\frac{18}{7})^3$

$=\frac{2}{3}n(517n-602)$.

$$(v)\ln\Pi_1(G_3)=2\sum_{u,v}\left(\frac{\ln d_u}{d_u}+\frac{\ln d_v}{d_v}\right)$$

$=|E_1|(2\frac{\ln 2}{4}+2\frac{\ln 2}{4})+|E_2|(2\frac{\ln 4}{4}+2\frac{\ln 4}{4})$

$=12n(2\frac{\ln 3}{3}+2\frac{\ln 3}{3})+(18n^2-12n)(2\frac{\ln 3}{6}+2\frac{\ln 3}{6})$

$=13.1689n^2$.

$$(vi)\ln\Pi_2(G_3)=\sum_{u,v}\ln(d_u+d_v)$$

$=|E_1|\ln(2+4)+|E_2|\ln(4+4)$

$=12n\ln(2+4)+(18n^2-12n)\ln(4+4)$

$=3.4512n(10.8453n-1)$.

$$(vii)\ln\Pi_1^*(G_3)=\sum_{u,v}\ln d_u+\ln d_v$$

$=|E_1|(\ln 2+\ln 4)+|E_2|(\ln 4+\ln 4)$

$=12n(\ln 2+\ln 4)+(18n^2-12)(\ln 4+\ln 4)$

$=n(49.9068n-8.3112)$.

Now we present the results for Sheet Silicate shown in Fig4a.

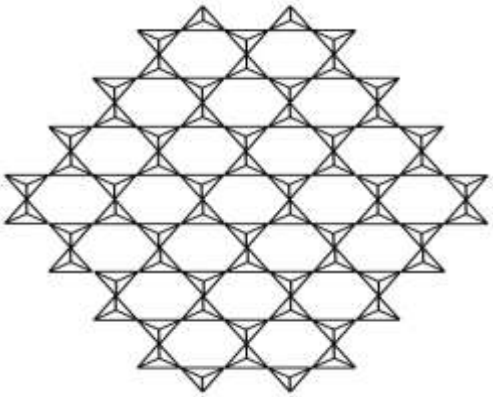

Fig4a: Sheet Silicate SL_n with $n=3$

Remark 2.4. We now consider the molecular graph $G_3=SL_n$, Figure 4. It is easy to see that $|V(G_4)|=15n^2+3n$ and $|E(G_4)|=36n^2$. We partition the edges of G_4 into three subsets $E_1(G_4)$, $E_2(G_4)$ and twtypes of edges.

(d_u,d_v) where $uv\in E(G)$	$E_1=[3,3]$	$E_2=[3,6]$	$E_3=[6,6]$
Number of edges	$6n$	$18n^2+6n$	$18n^2-12n$

Table 4: Edge partition of Sheet Silicate Network SL_n based on degrees of end vertices of each edge.

$E_3(G_4)$. Table 4 shows the number of two types of edges.

Theorem 2.4. Consider the graph G_4 of Sheet Silicate SL_n. Then

$$(i) M_1(G_4) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$= |E_1|(3+3) + |E_2|(3+6) + |E_3|(6+6)$$

$$= 6n(3+3) + (18n^2 + 6n)(3+6) + (18n^2 - 12n)(6+6)$$

$$= 54n(7n-1)$$

$$(ii) M_2(G_4) = \sum_{uv \in E(G)} (d_u \times d_v)$$

$$= |E_1|(3\times 3) + |E_2|(3\times 6) + |E_3|(6\times 6)$$

$$= 6n(3\times 3) + (18n^2 + 6n)(3\times 6) + (18n^2 - 12n)(6\times 6)$$

$$= 54n(18n-5)$$

$$(iii) mM_4(G_4) \le nM_2(G_4)$$

$$(36n^2)(54n(7n-1)) \le (15n^2 + 3n)(54n(18n-5)), \text{ for } n \ge 2$$

$$(iv) AZI(G_4) = \sum_{u,v} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

$$= |E_1|\left(\frac{9}{4}\right)^3 + |E_2|\left(\frac{18}{7}\right)^3 + |E_3|\left(\frac{36}{10}\right)^3$$

$$= 6n\left(\frac{9}{4}\right)^3 + (18n^2 + 6n)\left(\frac{18}{7}\right)^3 + (18n^2 - 12n)\left(\frac{36}{10}\right)^3$$

$$= 104976n^2\left(\frac{468}{42875}\right) + 2187n\left(\frac{1}{32} - \frac{32}{125} + \frac{16}{343}\right)$$

$$(v) \ln \Pi_1(G_4) = 2\sum_{u,v} \left(\frac{\ln d_u}{d_u} + \frac{\ln d_v}{d_v}\right)$$

$$= |E_1|\left(2\frac{\ln 3}{3} + 2\frac{\ln 3}{3}\right) + |E_2|\left(2\frac{\ln 3}{6} + 2\frac{\ln 3}{6}\right) + |E_3|\left(2\frac{\ln 6}{6} + 2\frac{\ln 6}{6}\right)$$

$$= 6n\left(2\frac{\ln 3}{3} + 2\frac{\ln 3}{3}\right) + (18n^2 + 6n)\left(2\frac{\ln 3}{6} + 2\frac{\ln 3}{6}\right) + (18n^2 - 12n)\left(2\frac{\ln 6}{6} + 2\frac{\ln 6}{6}\right)$$

$$= 2.4318n(18.6847n + 1)$$

$$(vi) \ln \Pi_2(G_4) = \sum_{u,v} \ln(d_u + d_v)$$

$$= |E_1| \ln(3+3) + |E_2| \ln(3+6) + |E_3| \ln(6+6)$$

$$= (6n)\ln(3+3) + (18n^2 + 6n)\ln(3+6) + (18n^2 - 12n)\ln(6+6)$$

$$= 5.8850n(14.3209n - 1)$$

$$(vii) \ln \Pi_1^*(G_4) = \sum_{u,v} \ln d_u + \ln d_v$$

$$= |E_1|(\ln 3 + \ln 3) + |E_2|(\ln 3 + \ln 6) + |E_3|(\ln 6 + \ln 6)$$

$$= 6n(\ln 2 + \ln 2) + (18n^2 + 6n)(\ln 2 + \ln 4) + (18n^2 - 12n)(\ln 4 + \ln 4)$$

$$= 12.4767n(9.3398n - 1)$$

3 Conclusion and general remarks

In this paper, certain degree based topological indices, general Zagreb, Zagreb inequality, augmented Zagreb, logarithm of first, second and modified first multiplicative Zagreb indices for Chain Oxide COX_n, Chain Silicate CS_n, Sheet Oxide OX_n and Sheet Silicate SL_n molecular structures were studied for the first

time and analytical closed formulae were determined for these structures which will help the people working in network science to understand the underlying topologies of these structures.

The readers may consider these structures for distance based topological descriptors for future studies.

References

1. Amic, D.; Beslo, D.; Lucic, B.; Nikolic, S.; Trinajstić N., The vertex-connectivity index revisited, *J. Chem. Inf. Comput. Sci*. **38,** 819-822, (**1998**).

2. Baig, A. Q.; Imran, M.; Ali, H., Computing Omega, Sadhana and PI Polynomial of Benzoid Carbon Nanotubes, *OAM-RC*, **9,** 248-255, (**2015**).

3. Baig, A. Q.; Imran, M.; Ali, H.; Rehman, S. U., Computing topological polynomials of certain nanostructures, *JOAM.*, **17,** 877-883, (**2015**).

4. Baig, A. Q.; Imran, M.; Ali, H., On topological indices of poly oxide, poly silicate, DOX, and DSL networks, *Can. J. Chem.,*. **93,** 730-739, (**2015**).

5. Bollobás, B.; Erdös, P., Graphs of extremal weights, *Ars Combinatoria*, **50,** 225-233, (**1998**).

6. Caporossi, G.; Gutman, I.; Hansen, P.; Pavlovc, L., Graphs with maximum connectivity index, *Comput. Bio. Chem.*, **27,** 85-90, (**2003**).

7. Diudea, M. V.; Gutman, I.; Lorentz, J., Molecular Topology, Nova, Huntington, (**2001**).

18. Wiener, H., Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.*, . ***69,** 17-20, **(1947)**.*

19. Chakraoui M.; El Kalay A., Local Parallel Index(LPI) in Databases System, *MAGNT Research Report*, **3(1)**, 23-32, (2015).

8. Furtula, B.; Graovac, A.; Vukičević, D., *J. Math. Chem.*, **48,** 370, (**2010**).

9. Gutman, I.; Polansky, O. E., Mathematical concepts in organic chemistry, Springer-Verlag, New York, (**1986**).

10. Hansen P.; and Vukičević, D., *Croat. Chem. Acta*, **80,** 165, (**2007**).

11. Hayat, S.; Siddiqui, H. M. A., On bipartite edge frustration of carbon and boron nanotubes, *Studia UBB chimia*, *LXI*, **1,** 283-290, (**2016**).

12. Hayat, S.; Imran, M., Computation of topological indices of certain networks, *Appl. Math. Comput.*, **240,** 213-228, (**2014**).

13. Hu, Y.; Li, X.; Shi, Y.; Xu, T.; Gutman, I., On molecular graphs with smallest and greatest zeroth-order general Randi c′ index, *MATCH Commun. Math. Comput. Chem.*, **54,** 425-434, (**2005**).

14. Imran, Muhammad; Baig, Abdul Qudair; Ali, Haidar, On molecular topological properties of hex-derived networks, *J. Chemometrics*, **30,** 121-129, (**2016**).

15 Imran, Muhammad; Baig, Abdul Qudair; Ali, Haidar, On topological properties of dominating David derived networks, *Can. J. Chem.*, **94,** 137-148, (**2016**).

16. Li, X.; Gutman, I., Mathematical aspects of Randi c′ -type molecular structure descriptors, mathematical chemistry monographs No. 1 , Kragujevac (**2006**).

17. Randić, M., On Characterization of molecular branching, *J. Amer. Chem. Soc.*, **97,** 6609-6615, (**1975**).