Study of The Paraline Graphs of Certain Benzenoid Structures Using Topological Indices

Zeeshan Saleem Mufti[1*], [2]Sohail Zafar*, [2]Zohaib Zahid, Faisal Nadeem[1]

[1]Department of Mathematics, Comsats Institute of Information Technology, Lahore.
[2]University of Management and Technology (UMT), Lahore Pakistan.

Abstract: Topological indices are valuable in the study of QSAR/QSPR. There are numerous applications of graph theory in the field of structural chemistry. In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, ABC_4, and GA_5 indices of the paraline graphs of triangular and linear parallelogram Benzenoid structures.

Keywords: Topological indices, Paraline graph, Triangular Benzenoid, Parallelogram Benzenoid**.**

1. Introduction

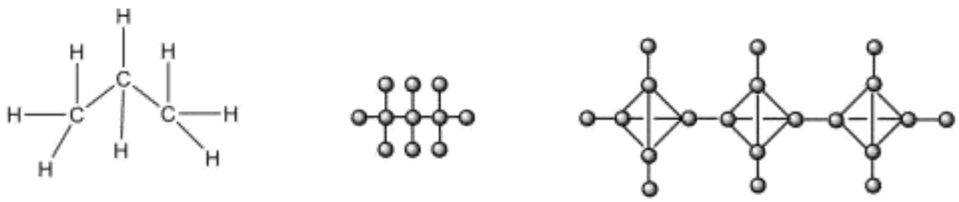
Consider G is simple graph having vertex set $V(G)$ and edge set $E(G)$. For any vertex u, N_u represents its neighbours set in G, $|N_u|$ is the degree d_u of vertex u, $S_u = \sum_{v\in N_u} d_v$ and $K(u)$ is the complete graph on vertex set N_u. If we replace each edge of a graph G by a path of length 2 then the resulting graph is known as subdivision graph $S(G)$. The line graph $L(G)$ is the graph whose vertices are the edges of G, two vertices e and f are incident if and only if they have a common end vertex in G. The paraline graph of G is the line graph of subdivision graph of G which will be denoted by G^*. There is another way to build G^* from G as follows:

1. Substitute every vertex $u \in V(G)$ by $K(u)$;
2. Join by edge all vertices of $K(u_1)$ with all vertices of $K(u_2)$ in G^* if and only if there is an edge between u_1 and u_2 in G;
3. For each vertex v of $K(u)$, degree of v in G^* is same as the degree of u in G.

Paraline graphs are very important in structural chemistry, but still in the last few decades they were considered very little in chemical graph theory. A molecular graph is a collection of points indicating the atoms in the molecule and set of lines indicating the covalent bonds. For example, consider the Hydrocarbon C_3H_8, its molecular structure and molecular graph is shown in Fig. 1 (a) and (b). However, there are other ways to attach graph with molecules, for instance a smallest collection of localized orbitals each reprsented by a vertex, with edges described the stronger connections among pairs of orbitals. In fact, such graphs were understood in some early quantum chemical mechanisms. The vertices of Paraline graphs of a molecular graph correspond to its atomic hybrid orbitals, and their edges corresponds to stronger interactions among pairs of these orbitals. Paraline graph of a molecular graph of Hydrocarbon C_3H_8, is Shown in Fig. 1. In structural chemistry and biology, molecular structure descriptors are utilized for modeling information of molecules, which are known as topological indices. Many topological indices are introduced to explain the physical and chemical properties of molecules [1, 2]. Topological indices are generally divided into three categories: degree-based indices [3, 4, 5, 6], distance-based indices [7, 8, 9, 10, 11, 12], and spectrum-based indices [13, 14, 15]. There are also some topological indices based on both degrees and distances (see [16, 17, 18]).

For futher study on degree based topological indices see [31, 32, 33, 34].

The general Randić index of G is introduced in [19].



(a) (b) (c)

Figure 1

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

where α is a real number. Then $R_{-1/2}(G)$ is known as Randic index of G.
The first general Zagreb index is introduced by Li and Zhao in [20]:

$$M_{\alpha}(G) = \sum_{u \in V(G)} (d_u)^{\alpha}. \quad (2)$$

In 2010, general sum-connectivity index $\chi_{\alpha}(G)$ has been introduced in [21]:

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha}. \quad (3)$$

Estrada et al. initiated the atom-bond connectivity (*ABC*) index in [22] which is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (4)$$

D. Vukicevic and B. Furtula introduced the geometric arithmetic (*GA*) index in [23] which is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \quad (5)$$

The fourth member of the class of *ABC* index was given by M. Ghorbani et al. in [24] as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \quad (6)$$

Graovac et al. Introduced the 5th *GA* index in [25] as

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \quad (7)$$

2. Topological Indices Of Paraline Graphs

In 2011, Ranjini et al. calculated the explicit expressions for the Shultz index of the subdivision graph of the ladder, wheel, helm and tadpole graphs [26]. They also studied the Zagreb indices of the paraline graphs of the ladder, wheel and tadpole graphs in [27]. In 2015, Su and Xu calculate the general sum-connectivity index and co-index of the paraline graphs of the ladder, wheel and tadpole graphs in [28]. In [29], Nadeem et al. computed ABC_4 and GA_5 indices of the paraline graphs of the ladder, wheel and tadpole graphs. They also studied generalized Randic, general Zagreb, general sum-connectivity, *ABC*, *GA*, ABC_4 and GA_5 indices of the paraline graphs of 2D-lattice, nanotube and nanotorus $TUC_4C_8[p,q]$ in [30].
In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, *ABC*, *GA*, ABC_4 and GA_5 indices of the paraline graphs of triangular and linear parallelogram benzenoid structures.
In order to calculate the number of edges of the line graph, the following lemma is important for us.

Lemma 2.1. Let G be a graph. Then $|E(L(G))| = \sum_{u \in V(G)} \frac{d_u^2}{2} - |E(G)|$ where $L(G)$ is the line graph of G.

3. Results and discussion.

3.1 Topological Indices Of The Paraline Graph Of Triangular Benzenoid.

The molecular graph of triangular benzenoid is shown in Fig. 2 and is denoted by T_n. There are n^2+4n+1 vertices and $\frac{3(n^2+3n)}{2}$ edges in T_n.

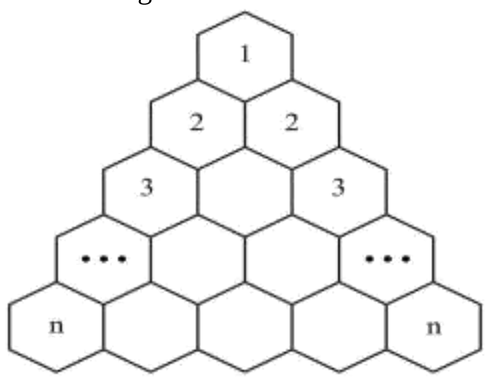


Figure 2. Triangular Benzenoid

Theorem 3.1. Let G^* be the Paraline graph of T_n. Then

$$M_\alpha(G^*) = 2^{\alpha+1}(3n+3) + 3^{\alpha+1}(n^2+n-2).$$

Proof The graph G^* is shown in Fig. 3. In G^* there are total $3(n^2+3n)$ vertices among which $6(n+1)$ vertices are of degree 2 and $3(n^2+n-2)$ vertices are of degree 3. Hence we get $M_\alpha(G^*)$ by using Formula (2).

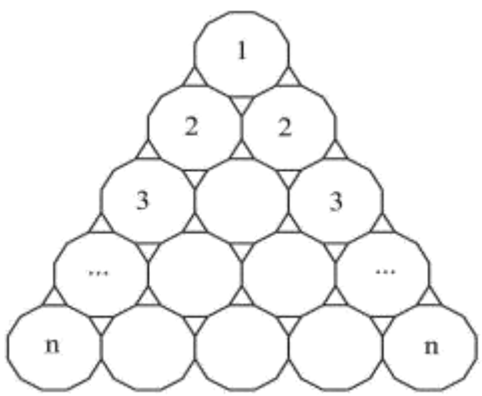


Figure 3. Paraline graph of Triangular Benzenoid

Theorem 3.2. Let G^* be the Paraline graph of T_n. Then

1. $R_\alpha(G^*) = 4^\alpha(3n+9) + 6^{\alpha+1}(n-1) + \frac{3}{2}9^\alpha(3n+4)(n-1)$;
2. $\chi_\alpha(G^*) = 4^\alpha(3n+9) + 5^\alpha(6n-6) + \frac{3}{2}6^\alpha(3n+4)(n-1)$;
3. $ABC(G^*) = 3n^2 + \left(\frac{9\sqrt{2}}{2}+1\right)n + \frac{3\sqrt{2}}{2} - 4$;
4. $GA(G^*) = \frac{9}{2}n^2 + \left(\frac{12\sqrt{6}}{5}+\frac{9}{2}\right)n + 3 - \frac{12\sqrt{6}}{5}$.

Proof: The subdivision graph $S(T_n)$ contains $3n^2+9n$ edges and $\frac{1}{2}(5n^2+17n+2)$ vertices among which $\frac{1}{2}(3n^2+15n+6)$ vertices are of degree 2 and remaining n^2+n-2 vertices are of degree 3. Hence, by Lemma 2.1 the total number of edges of G^* are $\frac{1}{2}(9n^2+21n-6)$. The edge set $E(G^*)$ divides into three edge partitions based on degrees of the end vertices, i.e. $E(G^*)=E_1(G^*)\cup E_2(G^*)\cup E_3(G^*)$. The edge partition $E_1(G^*)$ contains $3n+9$ edges uv, where $d_u=d_v=2$, the edge partition $E_2(G^*)$ contains $6n-6$ edges uv, where $d_u=2$ and $d_v=3$, and the edge partition $E_3(G^*)$ contains $\frac{3}{2}(3n+4)(n-1)$ edges uv, where $d_u=d_v=3$. From Formulas (1), (3), (4) and (5), we obtain the required results.

Theorem 3.3. Let G^* be the Paraline graph of T_n. Then

1. $ABC_4(G^*)=2n^2+\left(\frac{6\sqrt{2}}{5}+\frac{3\sqrt{110}}{10}+\frac{3\sqrt{14}}{8}+\frac{\sqrt{30}}{2}-\frac{10}{3}\right)n+\frac{9\sqrt{6}}{4}+\frac{3\sqrt{35}}{5}-\frac{12\sqrt{2}}{5}-\frac{3\sqrt{110}}{10}-\frac{3\sqrt{14}}{8}-\frac{\sqrt{30}}{2}+\frac{4}{3}$;

2. $GA_5(G^*)=\frac{9}{2}n^2+\left(\frac{24\sqrt{10}}{13}-\frac{3}{2}+\frac{72\sqrt{2}}{17}\right)n+\frac{8\sqrt{5}}{3}-\frac{24\sqrt{10}}{13}-\frac{72\sqrt{2}}{17}+3.$

Proof The edge set $E(G^*)$ can be divided into seven edge partitions $E_i(G^*)$, $i=4,5,\ldots,10$, i.e. $E(G^*)=\cup_{i=4}^{10}E_i(G^*)$ depending on the degree sum of neighbors of end vertices. The edge partition $E_4(G^*)$ contains 9 edges uv, where $S_u=S_v=4$, the edge partition $E_5(G^*)$ contains 6 edges uv, where $S_u=4$ and $S_v=5$, the edge partition $E_6(G^*)$ contains $3n-6$ edges uv, where $S_u=S_v=5$, the edge partition $E_7(G^*)$ contains $6n-6$ edges uv, where $S_u=5$ and $S_v=8$, the edge partition $E_8(G^*)$ contains $3n-3$ edges uv, where $S_u=S_v=8$, the edge partition $E_9(G^*)$ contains $6n-6$ edges uv, where $S_u=8$ and $S_v=9$, and the edge partition $E_{10}(G^*)$ contains $\frac{3}{2}(n-1)(3n-2)$ edges uv, where $S_u=S_v=9$. From Formulas (6) and (7), we obtain the required results.

4. Topological Indices Of The Paraline Graph Of Linear Parallelogram Benzenoid.

The molecular graph of linear parallelogram benzenoid is shown in Fig. 4 and is denoted by $P_{m,n}$. There are $2mn+2m+2n$ vertices and $3mn+2n+2m-1$ edges in $P_{m,n}$.

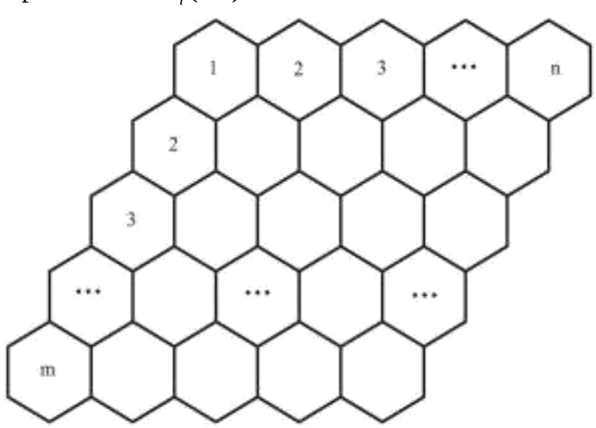


Figure 4. Linear parrallelogram Benzenoid

Theorem 4.1. Let G^* be the Paraline graph of $P_{m,n}$.Then $M_\alpha(G^*) = 2^{\alpha+2}(m+n+1) + 3^{\alpha+1}(2mn-2)$.

Proof The graph G^* is shown in Fig. 5. In G^* there are total $6mn+4m+4n-2$ vertices among which $4m+4n+4$ vertices are of degree 2 and $6mn-6$ vertices are of degree 3. Hence we get $M_\alpha(G^*)$ by using the Formula (2).

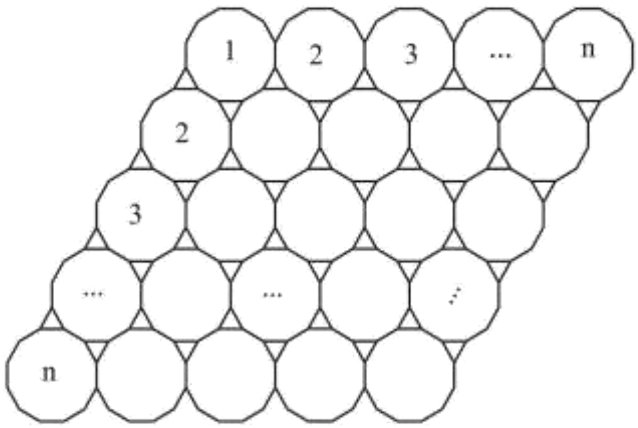


Figure 5. Paraline graph of Linear parallelogram Benzenoid

Theorem 4.2. Let G^* be the Paraline graph of $P_{m,n}$. Then

1) $R_\alpha(G^*) = 4^\alpha(2m+2n+8) + 6^\alpha(4m+4n-8)$ $+9^\alpha(9mn-2m-2n-5)$

;

2) $\chi_\alpha(G^*) = 4^\alpha(2m+2n+8) + 5^\alpha(4m+4n-8) +$ $6^\alpha(9mn-2m-2n-5)$

3) $ABC(G^*) = \left(6m + 3\sqrt{2} - \frac{4}{3}\right)n + \left(3\sqrt{2} - \frac{4}{3}\right)m - \frac{10}{3}$;

4) $GA(G^*) = \left(9m + \frac{8\sqrt{6}}{5}\right)n + \frac{8\sqrt{6}}{5}m + 3 - \frac{16\sqrt{6}}{5}$.

Proof The subdivision graph $S(P_{m,n})$ contains $6mn+4m+4n-2$ edges and $5mn+4m+4n-1$ vertices among which $3mn+4m+4n+1$ vertices are of degree 2 and remaining $2mn-2$ vertices are of degree 3. Hence, by Lemma the total number of edges of G^* are $9mn+4m+4n-5$. The edge set $E(G^*)$ divides into three edge partitions based on degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge partition $E_1(G^*)$ contains $2m+2n+8$ edges uv, where $d_u = d_v = 2$, the edge partition $E_2(G^*)$ contains $4m+4n-8$ edges uv, where $d_u = 2$ and $d_v = 3$, and the edge partition $E_3(G^*)$ contains $9mn-2m-2n-5$ edges uv, where $d_u = d_v = 3$. From Formulas (1), (3), (4) and (5), we obtain the required results.

Theorem 4.3. Let G^* be the Paraline graph of $P_{m,n}$. Then

1. $ABC_4(G^*) = \left(4m + \frac{4\sqrt{2}}{5} + \frac{\sqrt{14}}{4} + \frac{\sqrt{110}}{5} + \frac{\sqrt{30}}{3} - \frac{32}{9}\right)n +$ $\left(\frac{4\sqrt{2}}{5} + \frac{\sqrt{14}}{4} + \frac{\sqrt{110}}{5} - \frac{32}{9} + \frac{\sqrt{30}}{3}\right)m$ $-\frac{\sqrt{14}}{2} + 2\sqrt{6} + \frac{4\sqrt{35}}{5} - \frac{16\sqrt{2}}{5} - \frac{2\sqrt{110}}{5} - \frac{2\sqrt{30}}{3} + \frac{28}{9}$;

2. $GA_5(G^*) = \left(9m + \frac{48\sqrt{2}}{17} - 4 + \frac{16\sqrt{10}}{13}\right)n + \left(\frac{16\sqrt{10}}{13} - 4 + \frac{48\sqrt{2}}{17}\right)m + 3 + \frac{32\sqrt{5}}{9} - \frac{96\sqrt{2}}{17} - \frac{32\sqrt{10}}{13}$.

Proof The edge set $E(G^*)$ can be divided into seven edge partitions $E_i(G^*)$, $i = 4,5,\ldots,10$, i.e. $E(G^*) = \cup_{i=4}^{10} E_i(G^*)$ depending on the degree sum of neighbors of end vertices . The edge partition $E_4(G^*)$ contains 8 edges uv, where $S_u = S_v = 4$, the edge partition $E_5(G^*)$ contains 8 edges uv, where $S_u = 4$ and $S_v = 5$, the edge partition $E_6(G^*)$ contains $2m+2n-8$ edges uv, where $S_u = S_v = 5$, the edge partition $E_7(G^*)$ contains $4m+4n-8$ edges uv , where $S_u = 5$ and $S_v = 8$, the edge partition $E_8(G^*)$ contains $2m+2n-4$ edges uv, where $S_u = S_v = 8$, the edge partition $E_9(G^*)$ contains $4m+4n-8$ edges uv, where $S_u = 8$ and $S_v = 9$, and the edge partition $E_{10}(G^*)$ contains $9mn-8m-8n+7$ edges uv, where $S_u = S_v = 9$. From Formulas (6) and (7), we obtain the required results.

5. Conclusion

In this paper, generalized Randic, general Zagreb, general sum-connectivity, *ABC*, *GA*, ABC_4 and GA_5 indices for paraline graphs of triangular and linear parallelogram benzenoid structures were studied.

References

1. Randic, M.; On characterization of molecular branching. *J. Am. Chem. Soc.* 97, 6609-6615 (1974).
2. Wiener, H.J.; Structural Determination of Para_n Boiling Points. *J. Amer. Chem. Soc.* 69, 17-20 (1947).
3. Li, X.; Shi, Y.; A survey on the Randi_c index. *MATCH Commun. Math. Comput. Chem.* 59(1),127-156 (2008).
4. Li, X.; Shi, Y.; Wei, M.; Li, J. On a conjecture about tricyclic graphs with maximal energy. *MATCH Commun. Math. Comput. Chem.* 72(1), 183-214 (2014).
5. Rada, J.; Cruz, R.; Vertex-degree-based topological indices over graphs. *MATCH Commun. Math. Comput. Chem.* 72, 603-616 (2014).
6. Yu, G.; Feng, L.; On connective eccentricity index of graphs. *MATCH Commun. Math. Comput. Chem.* 69, 611-628 (2013).
7. Fozan-AL.; Manuel, T.P.; Rajasingh, I.; Rajan, R.; Computing Szeged index of certain nano sheets using partition technique. *MATCH Commun. Math. Comput. Chem.* 72, 339-353 (2014).
8. Azari, M. Iranmanesh, A.; Harary index of some nano-structures. *MATCH Commum. Math. Com-put. Chem.* 71, 373-382 (2014) .
9. Feng, L.; Liu, W.; Yu, G.; Li, S.; The hyper-Wiener index of graphs with given bipartition. *Utilitas Math.* 95, 23-32 (2014).
10. Hosseini, S.; Ahmadi, M.; Gutman, I.; Kragujevac trees with minimal atom-bond connectivity index.*MATCH Commun. Math. Comput. Chem.* 71, 5-20 (2014).
11. Knor, M.; Lu_zar, B.; _Skrekovski, R.; Gutman, I.; On Wiener index of common neighborhood graphs.*MATCH Commum. Math. Comput. Chem.* 72, 321-332 (2014).
12. Xu, K.; Liu, M.; Das, K.; Gutman, I.; Furtula, B.; A survey on graphs extremal with respect todistance-based topological indices. *MATCH Commun. Math. Comput. Chem.* 71, 461-508 (2014).
13. Das, K.; Sorgun, S.; On Randi_c energy of graphs. *MATCH Commun. Math. Comput. Chem.* 72,227-238 (2014).
14. Khosravanirad, A.; A lower bound for Laplacian Estrada index of a graph. *MATCH Commum.Math. Comput. Chem.* 70, 175-180 (2013).

15. Li, X.; Li, Y.; Shi, Y.; Gutman, I.; Note on the HOMO-LUMO index of graphs. *MATCH Commun.Math. Comput. Chem.* 70, 85-96 (2013).

16. Dehmer, M.; Emmert-Streib, F.; Grabner, M.; A computational approach to construct a multivariate complete graph invariant. *Inform. Sci.* 260, 200-208 (2014).

17. Feng, L.; Liu, W.; Ili_c, A.; Yu, G.; The degree distance of unicyclic graphs with given matching number. *Graphs Comb.* 29, 449-462 (2013).

18. Gutman, I.; Selected properties of the Schultz molecular topological index. *J. Chem. Inf. Comput.Sci.* 34, 1087-1089 (1994).

19. Bollobs, B.; Erds, P.; Graphs of extremal weights, *Ars Combin.* 50, (1998) 225-233.

20. Li, X.; Zhao, H.; Trees with the _rst three smallest and largest generalized topological indices.*MATCH Commun. Math. Comput. Chem.* 50, 57-62 (2004).

21. Zhou, B.; Trinajstic, N.; On general sum-connectivity index. *J. Math. Chem.* 47, 210-218 (2010).

22. Estrada, E.; Torres, L.; Rodriguez, L.; Gutman, I.; An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian J. Chem.*, 37A, 849-855 (1998).

23. Vukicevic, D.; Furtula, B.; Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* 46, 1369-1376 (2009).

24. Ghorbani, M.; Hosseinzadeh, M.A.; Computing ABC4 index of nanostar dendrimers. *Optoelectron.Adv. Mater. Rapid Commun.* 4(9), 1419-1422 (2010).

25. Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A.; Computing _fth geometric-arithmetic index for nanostar dendrimers. *J. Math. Nanosci* 1(1), 33-42 (2011).

26. Ranjini, P.S.; Lokesha, V.; Rajan, M.A.; n the Shultz index of the subdivision graphs. *Adv. Stud.Contemp. Math.* 21(3), 279-290 (2011).

27. Ranjini, P.S.; Lokesha, V.; Cangl, I.N.; On the Zagreb indices of the line graphs of the subdivision graphs. *Appl. Math. Comput.* 218, 699-702 (2011).

28. Su, G.; Xu, L.; Topological indices of the line graph of subdivision graphs and their Schur-bounds. *Appl. Math. Comput.* 253, 395-401 (2015).

29. Nadeem, M. F.; Zafar, S.; Zahid, Z.; Certain topological indicies of the line graph of subdivision graphs. *Appl. Math. Comput.* 271, 790-794 (2015).

30. Nadeem, M. F.; Zafar, S.; Zahid, Z.; On Topological properties of the line graph of subdivision graphs of certain nanostructures. *Appl. Math. Comput.* 273, 125-130 (2016).

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

32. Ali, H.; Siddiqui, H.M.A.; Shafiq, M.K.; On Degree-Based Topological Descriptors of Oxide and Silicate Molecular Structures. *MAGNT Research Report*,**4(4),** 135-142, 2016.

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

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