Kurdish Studies
January 2022
Volume: 10, No: 1, pp. 89-97
ISSN: 2051-4883 (Print) | ISSN 2051-4891 (Online)
www.KurdishStudies.net

DOI: 10.53555/ks.v10i1.3204

"Physical Analysis Of Subdivision Of Silicate Chain Graph Using Degree Based Topological Indices"

Veena M G[1*], Deepika T[2]

[1*]Research scholar, Dayananda Sagar University, Bangalore, (Assistant Professor Department of Mathematics, Govt. First Grade College Magadi), karnataka, India.
[2]Department of Mathematics, Dayananda Sagar University, Bangalore, Karnataka, India.

***Corresponding Author:** Veena M G
*Research scholar, Dayananda Sagar University, Bangalore, (Assistant Professor Department of Mathematics, Govt. First Grade College Magadi), karnataka, India.

Abstract
Minerals like silicon and oxygen set in tetrahedral $(Sio_4)^4$ units with different shapes of attachment are called silicates. Silicates are critical because from the chemical composition
of these elements we obtain the glass, ceramic, and cement. By sharing oxygen atoms on two corners of each tetrahedral, simple chain silicates are created. $[(Sio_3)_n]^2\ n$ is the generic formula for cyclic silicate. In this work, we centralize on chain silicate graphs and find-out
multiple topological indices in view of edge dividing techniques. TIs such as Zagreb type TI, Geometric arithmetic index, Sum connectivity index, harmonic index, Inverse sum indeg index, Symmetric index division, SK indices. A graphical resemblance was also given to explore the behavior of the referred indices.

Key Words: Zagreb index, Inverse sum indeg index, Symmetric division index, SK index and Silicate graph

Introduction
Let G be a graph V(G) and E(G) represents a set of vertices and set of edges. The degree of the vertex is denoted as d_i where *i*(*G*) is the number of adjacent vertices of v, and edges of the graph G is the connection between u and v, will be represented as *e* = *uv*[10]. In order to predict the biological activities and characteristics of chemical compounds, quantitative structure activity (QSAR) and structure property relationship (QSPR) researchers

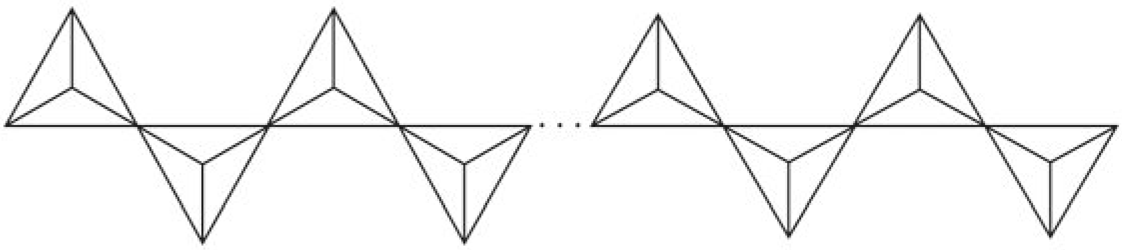


Figure 1: Silicate chain graph

now routinely use molecular structure descriptors[5]. A topological index is a quantity that is used to calculate characterize the chemical compound and predict certain physico-chemical properties like boiling point, molecular weight, density, refractive index[12].

Review of Literature
Zagreb Type Topological indices:
Gutman and Trinajsic first invented bi vertex degree topological indices, named as the first and second Zagreb index these indices are defined as[9][19]

$$M_1(G) = \sum_{(i,j)\epsilon E(G)} (d_i + d_j)$$
$$M_2(G) = \sum_{(i,j)\epsilon E(G)} (d_i * d_j)$$

New graph invariants called the third Zagreb index which is denoted as[8]

$$M_3(G) = \sum_{(i,j)\epsilon E(G)} |d_i * d_j|$$

Geeometric Arithmetic index:

The first GA- index was proposed by Vukicevic and Furtula[7]

$$GAI(G) = \sum_{(i,j)\epsilon E(G)} \frac{2\sqrt{d_i * d_j}}{d_i + d_j}$$

Sum connectivity index :

The sum connectivity index was proposed by Zhou and Trinajstic which is defined as for more information of these indices we go through to[3][4][13][20]

$$SCI(G) = \sum_{(i,j)\epsilon E(G)} \sqrt{\frac{1}{d_i + d_j}}$$

Harmonic index :

The Harmonic index H(G) is a vertex degree based topological index this index first appeared in [17] and was defined as[14][21]

$$H(G) = \sum_{(i,j)\epsilon E(G)} \frac{2}{d_i + d_j}$$

Inverse Sum Indeg Index :

Recently for extension and generalization of ISI index are also proposed [11].
The ISI index is defined as[1]

$$ISI(G) = \sum_{(i,j)\epsilon E(G)} \frac{d_i d_j}{d_i * d_j}$$

Symmetric division index :

SDD(G), or the symmetric division degree index of a graph, was first presented by Vukieevic and Gasperov in [6]. It is based on vertex degree and one of the 148 so-called Adriatic indices, and it has a strong ability to forecast the total surface area of polychlorobiphenyl

$$SDI(G) = \sum_{(i,j)\epsilon E(G)} \frac{{d_i}^2 + {d_j}^2}{d_i * d_j}$$

A useful and adaptable topological index, the symmetric division degree index has a greater quality than some of the more well-known VDB indices, particularly the geometric arithmetic index. Owing to the SDD's significance, numerous studies on this index have been carried out recently[2][15]

SK Index

Shegehalli and Kanabur proposed a new version of topological indices which are defined as[16][18]

$$SK(G) = \sum_{(i,j)\epsilon E(G)} \frac{d_i + d_j}{2}$$

$$SK_1(G) = \sum_{(i,j)\epsilon E(G)} \frac{d_i * d_j}{2}$$

$$SK_2\,(G) = \sum_{(i,j)\epsilon E(G)} (\frac{d_i * d_j}{2})^2$$

Results and Discussions:

Many graph theoretic techniques have been developed in the last few years for the investigation and prediction of molecular physico-chemical properties.
The aim of creating a topological index is to assign a numerical value to every chemical structure while maintaining the highest level of discrimination. Classifying structures and forecasting chemical and biological quantities are done with the help of these indices.
Topological indices are useful instruments in chemistry because they offer quick and easy method of quantifying a chemical compound's structural attribute. The graphical representation of the index makes chemical compounds easier to see chemical formula refer to figure 2, figure 3, figure 4, figure 5, figure 6, figure 7 and figure 8 and the general representation of chemical compounds as graphs and the use of topological indices to quantify various aspects of their structure provide a power full tool for the analysis, prediction and discovery of chemical compounds. These can help with interpretation of the results obtained from the topological indices and the identification of structural features that may be related to compounds

properties. Table 2, table 3, Table 4, Table 5, Table 6, Table 7 and Table 8 define the numerical comparison of computed results.

Vertex Edge Partition Of a Silicate Graph

Table-1

$(\alpha_i * \alpha_j)$	No of Edges
(3, 3)	n+5
(3, 6)	4n+2
(6, 6)	n-1

With the help of Table-1

$$M_1(G) = \sum_{(i,j)\epsilon E(G)} (\alpha_i + \alpha_j)$$

$$= (n+5)(3+3) + (4n+2)(3+6) + (n-1)(6+6)$$

$$M_2(G) = \sum_{(i,j)\epsilon E(G)} (\alpha_i . \alpha_j)$$

$$= (n+5)(3.3) + (4n+2)(3.6) + (n-1)(6.6)$$

$$M_3(G) = \sum_{(i,j)\epsilon E(G)} |\alpha_i - \alpha_j|$$

$$|(n+5)|3-3| + (4n+2)|3-6| + (n-1)|6-6|$$

$$GAI(G) = \sum_{(i,j)\epsilon E(G)} \frac{2\sqrt{\alpha_i * \alpha_j}}{\alpha_i + \alpha_j}$$

$$= (n+5).\frac{2\sqrt{3.3}}{3+3} + (4n+2).\frac{2\sqrt{3.6}}{3+6} + (n-1).\frac{2\sqrt{6.6}}{6+6}$$

$$SCI(G) = \sum_{(i,j)\epsilon E(G)} \sqrt{\frac{1}{\alpha_i + \alpha_j}}$$

$$= (n+5)\frac{1}{\sqrt{3+3}} + (4n+2)\frac{1}{\sqrt{3+6}} + (n-1)\frac{1}{\sqrt{6+6}}$$

$$H(G) = \sum_{(i,j)\varepsilon E(G)} \frac{2}{\alpha_i + \alpha_j}$$

$$= (n+5).\frac{2}{(3+3)} + (4n+2).\frac{2}{(3+6)} + (n-1)\frac{2}{(6+6)}$$

$$IS(G) = \sum_{(i,j)\epsilon E(G)} \frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}$$

$$= (n+5).\left(\frac{3.3}{3+3}\right) + (4n+2).\left(\frac{3.6}{3+6}\right) + (n-1).\left(\frac{6.6}{6+6}\right)$$

$$SDI(G) = \sum_{(i,j)\epsilon E(G)} \frac{\alpha^2{}_i + \alpha^2{}_j}{\alpha_i * \alpha_j}$$

$$= (n+5).\left(\frac{3^2+3^2}{3.3}\right) + (4n+2).\left(\frac{3^2+6^2}{3.6}\right) + (n-1).\left(\frac{6^2+6^2}{6.6}\right)$$

$$SK(G) = \sum_{(i,j)\epsilon E(G)} \frac{\alpha_i + \alpha_j}{2}$$

$$= (n+5).\left(\frac{3+3}{2}\right) + (4n+2).\left(\frac{3+6}{2}\right) + (n-1).\left(\frac{6+6}{2}\right)$$

$$SK_1(G) = \sum_{(i,j)\epsilon E(G)} \frac{\alpha_i . \alpha_j}{2}$$

$$= (n+5).\left(\frac{3.3}{2}\right) + (4n+2).\left(\frac{3.6}{2}\right) + (n-1).\left(\frac{6.6}{2}\right)$$

$$SK_1(G) = \sum_{(i,j)\epsilon E(G)} \left(\frac{\alpha_i + \alpha_j}{2}\right)^2$$

$$= (n+5).3^2 + (4n+2).\left(\frac{9}{2}\right)^2 + (n-1).6^2$$

Table 2: Comparison of $M_1(G), M_2(G), M_3(G)$

N	$M_1(G)$	$M_2(G)$	$M_3(G)$
1	86	162	18
2	140	279	30
3	194	396	42
4	248	513	54
5	302	630	66
6	356	747	78
7	410	864	90
8	464	981	102
9	518	1098	114
10	572	1215	126

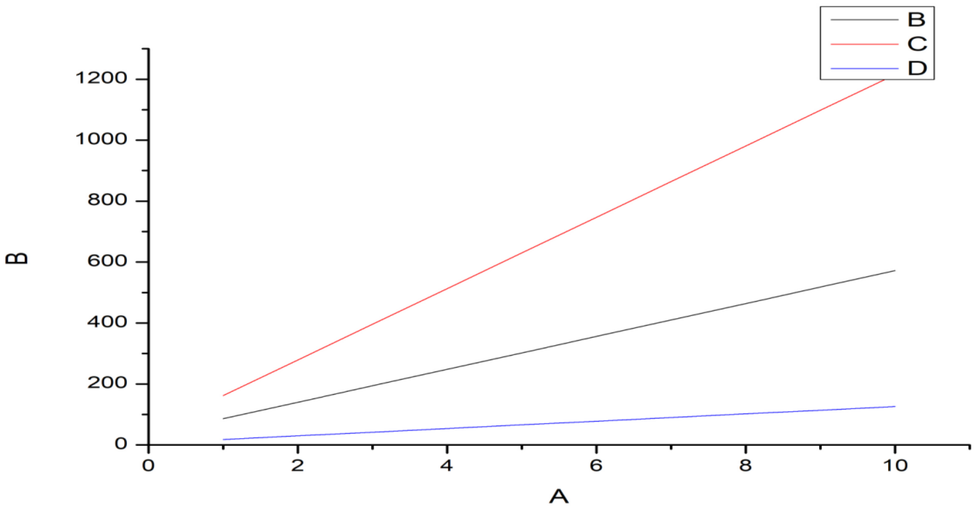


Figure 2: Graphical comparison of Zagreb type Index

Table 3: Numerical comparison of GA(G), SCI(G) , H(G), IS(G) ,SDI(G)

N	GA(G)	SCI(G)	H(G)	IS(G)	SDI(G)
1	11.6568	4.4472	3.3311	21	27
2	18.428	6.476	4.7198	33.5	41
3	25.1992	8.5048	6.1085	46	55
4	31.9704	10.5336	7.4972	58.5	69
5	38.7416	12.5624	8.8859	71	83
6	45.5128	14.5912	10.2746	83.5	97
7	52.284	16.62	11.6633	96	111
8	59.0552	18.6488	13.052	108.5	125
9	65.8264	20.6776	14.4407	121	139
10	72.5976	22.7064	15.8294	133.5	153

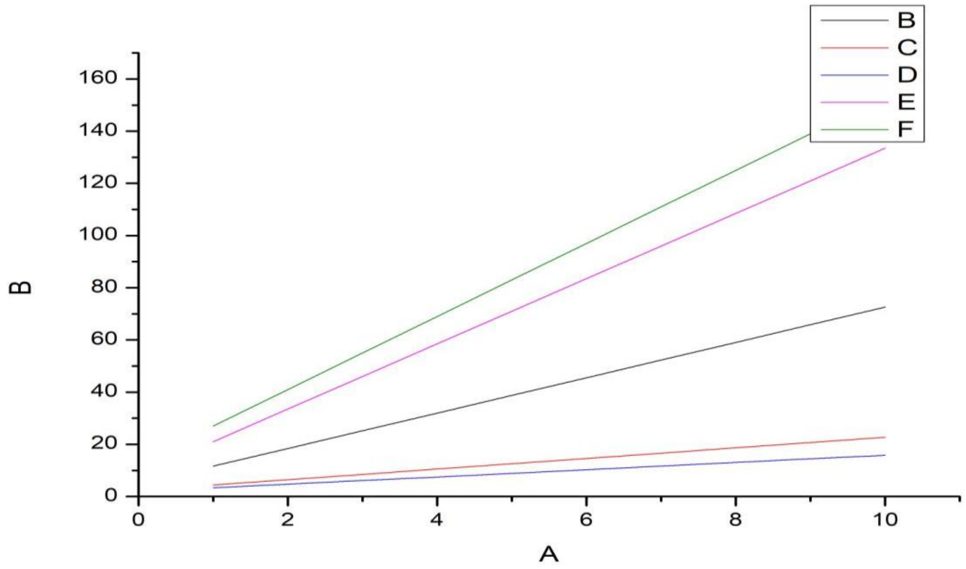


Figure 3: Graphical comparison of GA(G), SCI(G) , H(G), IS(G) ,SDI(G)

Table 4: Numerical comparison of $SK_1(G)$, SK_2 (G) , $SK_3(G)$

n	$SK_1(G)$	SK_2 (G)	$SK_3(G)$
1	27	99	175.5
2	54	158.1	301.5
3	81	157.5	427.5
4	108	275.7	553.5
5	135	333	679.5
6	162	391.5	805.5
7	189	450	931.5
8	216	508.5	10557.5
9	243	567	1183.5
10	270	625.5	1309.5

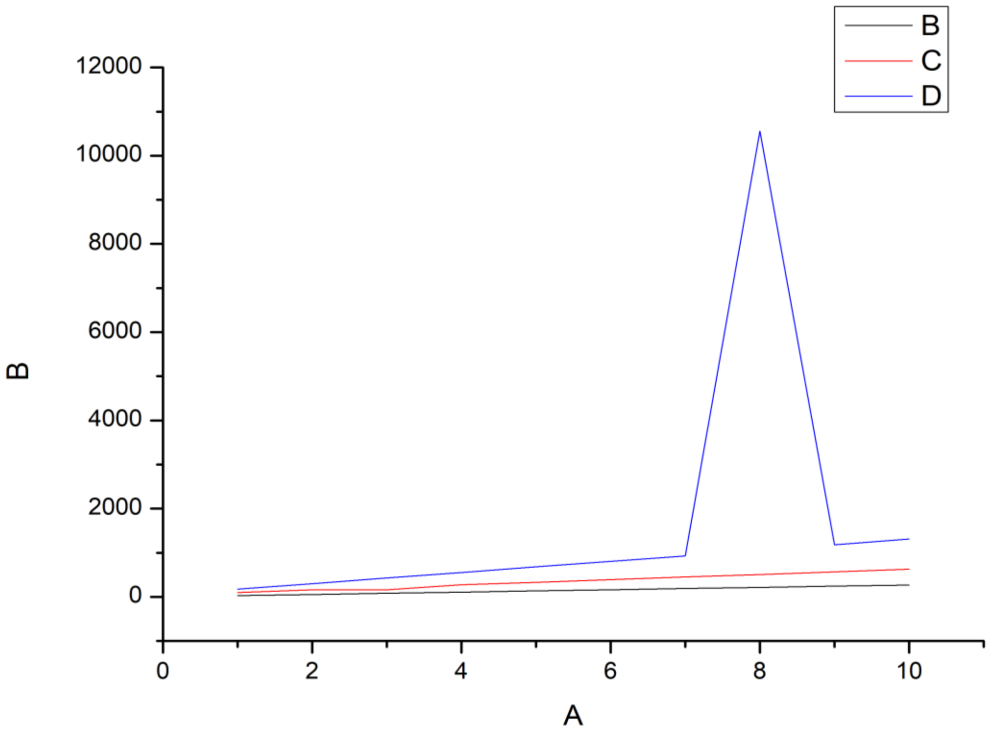


Figure 4: Graphical comparison of $SK_1(G)$, SK_2 (G) , $SK_3(G)$

Subdivision of Silicate graph

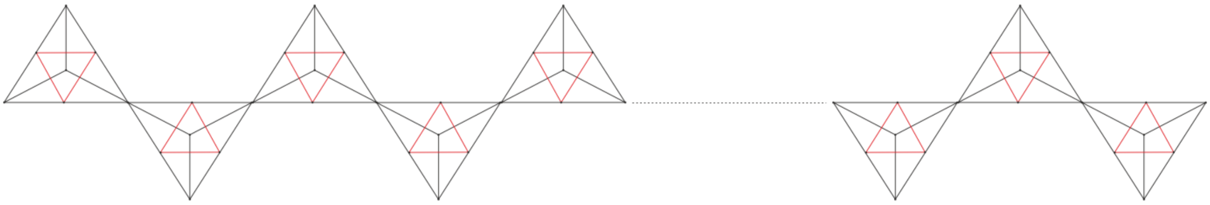


Figure 5

$(\alpha_i \,.\, \alpha_j)$	No of edges
(3,4)	2n + 45
(4, 4)	3n
(3 ,3)	n+2
(3, 6)	2n-2
(4, 6)	4n-4

$$M_1(G) = \sum_{(i,j)\epsilon E(G)} (\alpha_i + \alpha_j)$$

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

$$M_2(G) = \sum_{(i,j)\epsilon E(G)} (\alpha_i . \alpha_j)$$

$$= (2n + 4)(3.4) + 3n(4.4) + (n + 2)(3.3) + (2n - 2)(3.6) + (4n - 4)(4.6)$$

$M_3(G) = \sum_{(i,j)\epsilon E(G)} |(\alpha_i - \alpha_j)|$

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

$$GAI(G) = \sum_{(i,j)\epsilon E(G)} \frac{2\sqrt{\alpha_i . \alpha_j}}{\alpha_i + \alpha_j}$$

$$= (2n + 4).2\left(\frac{\sqrt{3.4}}{3 + 4}\right) + 3n.\,2\left(\frac{\sqrt{4.4}}{4 + 4}\right) + (2n - 2).2\left(\frac{\sqrt{3.6}}{3 + 6}\right) + (4n - 4).2\left(\frac{\sqrt{4.6}}{4 + 6}\right)$$

Table-6: Numerical comparison of subdivision of $MS_1(G)$, $MS_2(G)$, $MS_3(G)$

n	$MS_1(G)$	$MS_2(G)$	$MS_3(G)$
1	84	147	6
2	186	360	22
3	288	573	38
4	390	786	54
5	492	999	70
6	594	1212	86
7	696	1425	102
8	798	1638	118
9	900	1851	134
10	1002	2064	150

Figure 6: Graphical comparison of $MS_1(G)$, $MS_2(G)$, $MS_3(G)$

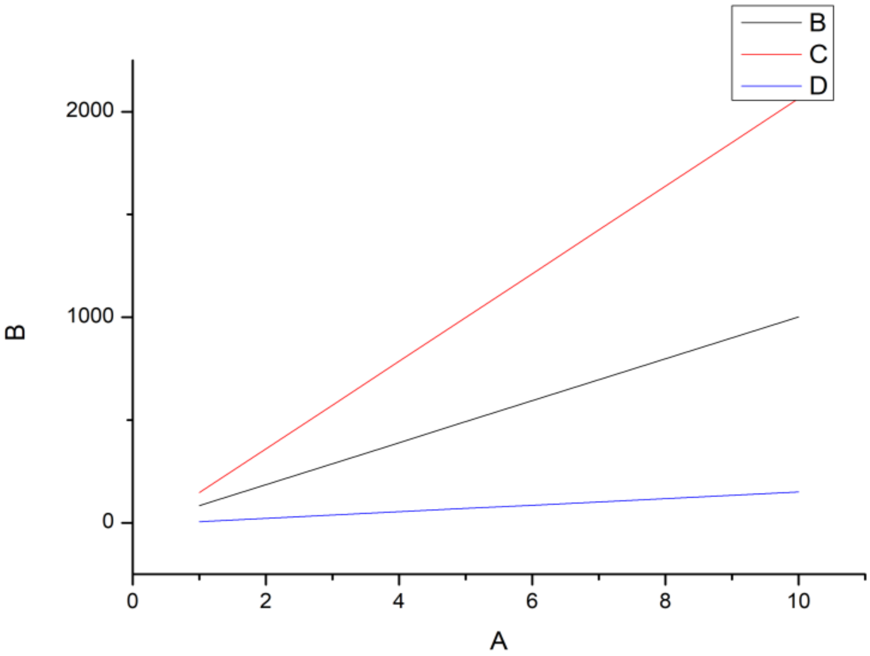


Table 7:Numerical Comparison of GAS(G), SCI(G), ISS(G), SDI(G), HS(G)

n	GAS(G)	SCI(G)	ISS(G)	SDI(G)	HS(G)
1	26.3076	3.6274	20.7858	18.5	2.3341
2	60.53	7.2942	41.7588	42.333	5.2332
3	94.7522	10.961	62.7318	71.3118	8.1323
4	128.9744	14.6278	83.7048	83.02	11.0314
5	163.1966	18.2946	104.6778	113.832	13.9305
6	197.4188	21.9614	125.6508	137.665	16.8296
7	231.641	25.6282	146.7716	161.498	19.7287
8	265.8632	29.295	167.5968	185.331	22.6278
9	300.0854	32.9618	188.5698	209.164	25.5269
10	334.3076	36.6286	209.5428	232.997	28.426

Figure 7: Graphical comparison of subdivision of GAS(G), SCI(G), ISS(G), SDI(G), HS(G)

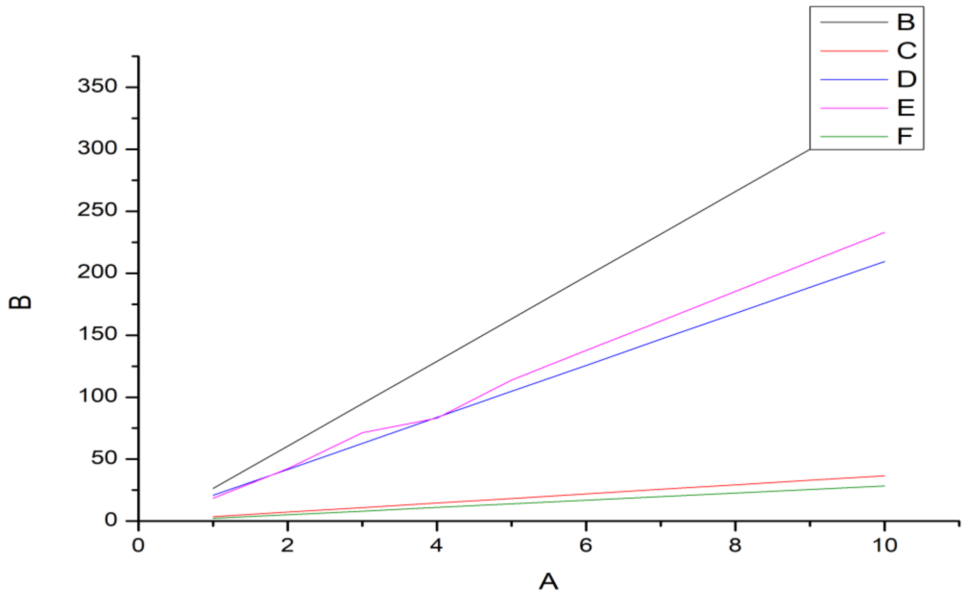
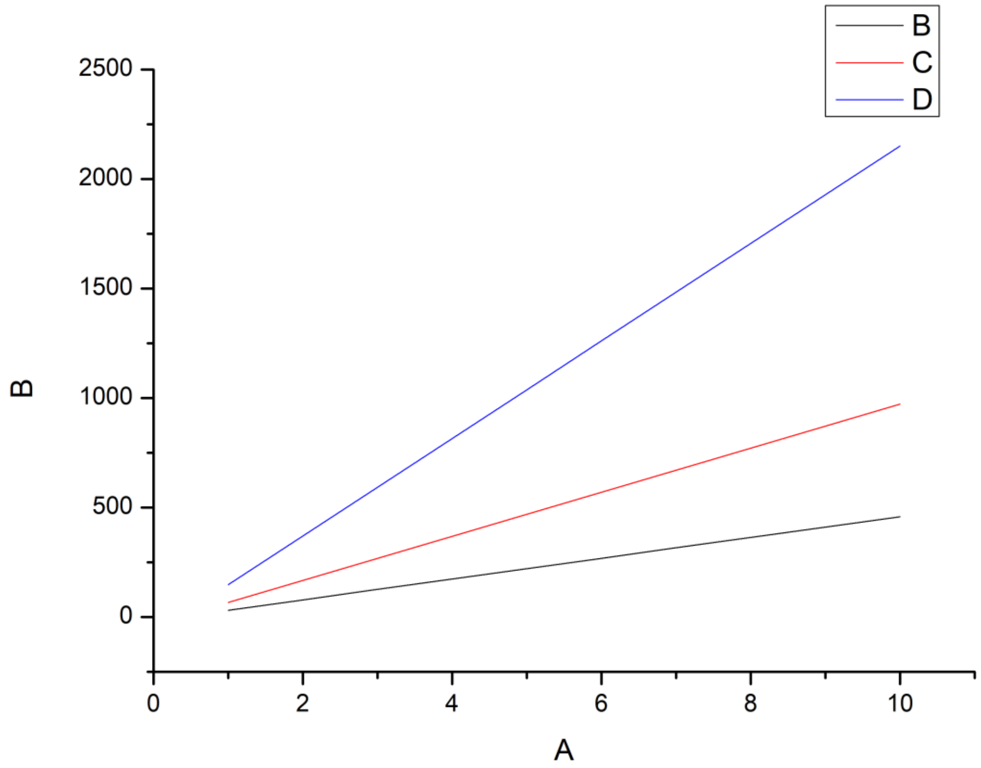


Table 8: Numerical comparison of $SK_1(G)$, $SK_2(G)$ and $SK_3(G)$

n	$SK_1(G)$	$SK_2(G)$	$SK_3(G)$
1	31.5	67.5	148.5
2	79	168	371
3	126.5	268.5	593.5
4	174	369	816
5	221.5	469.5	1038.5
6	269	570	1261
7	316.5	670.5	1483.5
8	364	771	1706
9	411.5	871.5	1928.5
10	459	972	2151

Figure 8 : Graphical comparison of $SK_1(G)$, $SK_2(G)$ and $SK_3(G)$



Conclusion : In this article we discussed on silicate chain graph and also subdivision of silicate chain graph by using various topological indices like Zagreb type topological index, Geometric Arithmetic index, Sum connectivity index, Harmonic index , Inverse sum in-deg index, Symmetric index division, SK indices and also study the behaviour of indices through a graphical comparison has also been provided.

References:

1. A. Doley, J.Buragohain, A.Bharali, Inverse sum in deg status index of graphs and its applications to octane isomers and benzenoid hydrocarbons, chemo metrics and intelligent laboratory system203, 104059, (2020), DOI:10.1016/j.chemo lab. 2020.104059.
2. B.Furtula, K.Das, I.Gutman, comparative analysis of symmetric division deg index as potentially useful molecular descriptor, Int.J Quantum chem 118(2018)2565
3. B.Zhou and N.Trinajstic, on a noval connectivity index. J.Math. Chem., 46(2009), 1252-12709.
4. B.Zhou and N.Trinajstic, on general sum connectivity inndex. J.Math. Chem., 47(1)(2010), 210-218
5. Diudo, M.V.;Gutman,I.;Lornetz, J.Molecular topology; Nova; Hunting, N Y, USA, 2001
6. D.Vukicevic, M.Gasperov, Bond additive modeling. 1. Adriatic indices, croat.chem. Acta 83(2010) 243-260
7. D.Vukicevic, B.Furtula, Topological index based on the ratio of geometrical and arithmetical means of end-vertex degree of edges, J.Math. chem 46(2009)1369-1376.
8. G.H. Fath-Tabar MATCH commun, Math. Comput. chem. 65(2011) 79-84 ISSN 0340-6253.
9. I. Gutman, N. Trinajstic, Graph theory and molecular orbits. Total π- electron energy of alternant hydrocarbons, chem, phys, lett.17(1972), 535- 538

10. I. Gutman and B. Furtula(eds). recent results in the theory of Randicindex, Univ. Kragujevac, Kragu-jevac, 2008
11. J. Buragohain, B.Deka, A.Bharali, A generalized ISI index of some chemical structures. Journal of molecular structure 1028, 127843,(2020). DOI:10.1016 lj. molstruc. 2020.127843.
12. Jia-Bao Liu, Haidar Ali, Muhammad Kashif Shafiq on Degree-Based Topological Indices of Symmetric chemical structure. Symmetry 2018, 10.619: DOI: 10,3390/sym10110619.
13. K.C Das, S.Das and B.Zhou, sum-connectivity index of a graph , Front, Math, China. 11(1)(2016), 47-54.
14. L. Zhong, the harmonic index for graphs, Appl. Math. Lett., 25(2012) 561-566.
15. Najaf Amraei Lavizan, Tehran, I.R.Iran, A survey on symmetric division degree index Journal of Discrete Mathematics and its Applications 8(2) (2023) 49-63.
16. Semiha Basdas, Nurkahh, serife Buyukkose A note on SK, SK1, SK2 indices of interval weighted graphs. Advances in Linear Algebra and Matrix theory 2021, 11, 14-20.
17. S. Fajtlowicz, on conjectures of Graffiti, II. Cong. Numer, 60(1987) 189-197.
18. Shigehalli, V. and Kanabur, R(2016) computing Degree-Based Topo;ogical indices of polyhex Nanotubes, Journal of Mathematical Nanoscience, 6, 47-55
19. T.Doslic, B. Furtula. A. Graovac, I Gutman, S.Moradi, Z.Yarahmadi, on vertex-degree-based molecular structure descriptors, MATCH commun, Math. comput. chem. 66(2011)613-626.
20. X. Li and I.Gutman, Mathematical aspects of Randic type molecular structure descriptors, Kragujevac(2006)
21. X. X_u, Relationships between harmonic index and other topological indices Appl. Math.Sci.,6(2012) 2013-2018