A COMPARATIVE STUDY ON DOMINATIONAL VARIANTS OF SOMBOR INDEX

Girish Sharma*   K. Bhuvaneswari**   Radha Rani V***
*Department of Mathematics, Mount Carmel College, Autonomous, Vasanthnagar, Bengaluru, Karnataka, India.
**Post Graduate Department of Mathematics, BMS College for Women (Autonomous), Bangalore, India.
***Department of Mathematics, NMKRV College, Jayanagar, Bengaluru, India.

Abstract
A Topological index functions as a molecular descriptor, allowing the physiochemical property of a chemical compound to be determined. There are degree-based, distance-based, and eccentricity-based topological indices. In this paper, we introduce the dominational variants of the Sombor index and investigate various predictive properties of the indices using a linear regression model.

This paper attempts to generalise the dominational-based topological index for a family of standard graphs by offering specific conclusions based on specific general graphs.

Keywords and phrases: Domination, Dominational degree, m-array tree, Status.

1. Introduction
A graph $G = (V, E)$ is a mathematical structure with elements of $V(G)$ being called as vertices or nodes and members of $E(G)$ are called as edges or lines. A topological index is a real valued function on the set of vertices of the graph.

Let us now look into various attributes associated with the vertices of a graph. The degree of a vertex v refers to the number of edges incident with a given vertex and is denoted as $d_G(v)$. The distance between any two vertices u and v in a graph is the length of the shortest path joining them, denoted by $d(u, v)$. The eccentricity of a vertex v is the distance of the farthest vertex from v and is given by $ecc(v) = \max\{d(u,v): v \in V(G)\}$. The radius *(r)* of a graph is the minimum of all the eccentricities of a vertex v. The status of a vertex v is the sum of the distance between v and all the remaining vertices of the graph G, denoted by $\sigma(v)$.

Weiner index was the first ever identified distance-based topological index, Randic index was the first ever identified degree-based topological index, and numerous topological indices have been identified in recent years. The important topological indices employed in this study are highlighted.
Gutman[1] proposed the Sombor index, which is related to the Euclidean norm, as provided by

$$SO(G) = \sum_{u,v \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}.$$

In light of the practical applications of the topological index, Kulli proposed the Nirmala index[2], denoted by
$$N(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}.$$
The HDR Nirmala index[2] is a topological index based on eccentricity, given by
$$HDRN(G) = \sum_{uv \in E(G)} \sqrt{d_{hr}(u) + d_{hr}(v)}.$$

Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

The HDR Sombor index [3] is another eccentricity-based topological index, defined as

$$HDRSO(G) = \sum_{uv \in E(G)} \sqrt{d_{hr}^2(u) + d_{hr}^2(v)}$$

where, $$d_{hr}(u) = \{v \in V(G): d(u,v) = r\}.$$

Ramane and Yalnaik[4] proposed a new distance-based topological index called as the sum-connectivity index, and used the same to calculate the boiling temperatures of specific benzenoid hydrocarbons by means of a linear regression model.

The status Sombor index[5] of a graph is defined as

$$SS(G) = \sum_{uv \in E(G)} \sqrt{\sigma(u)^2 + \sigma(v)^2}.$$

This paper attempts to combine the dominational concept of a graph and topological indices. A set $S \subseteq V(G)$ is said to be a dominating set if $N[S] = V$ where $N[S]$ represents the closed neighbourhood of $S.$ A dominating set with a minimum number of elements is called as a minimum dominating set and its cardinality gives the domination number $\Upsilon(G).$

We now define the dominational degree, dominational eccentricity and dominational status of a vertex. The dominational degree of a vertex is denoted as $D_G(v)$ and is given by

$$D_G(v) = |d_G(v) - \Upsilon(G)|.$$

The dominational eccentricity of a vertex is defined as follows:
$$D_{hr}(v) = |d_{hr}(v) - \Upsilon(G)|.$$

The dominational status of a vertex can be described by
$$D_\sigma(v) = |\sigma(v) - \Upsilon(G)|.$$

The following are some novel topological indices based on dominance.
Dominational Sombor index:

$$D_dSO(G) = \sum_{u,v \in E(G)} \sqrt{D_G^2(u) + D_G^2(v)},$$

Dominational HDR Sombor index:

$$D_{HDR}SO(G) = \sum_{uv \in E(G)} \sqrt{D_{hr}^2(u) + D_{hr}^2(v)},$$

Dominational Status Sombor index:

$$D_\sigma SO(G) = \sum_{uv \in E(G)} \sqrt{D_\sigma(u)^2 + D_\sigma(v)^2}.$$

The above defined topological indices are now generalized for certain standard graphs.

2. Certain Results on General graphs
Theorem 1: For any graph G, $D_dSO(G) \leq SO(G).$

Proof: Let $G = (p,q)$ be a graph with $\Delta(G) = \max\{d_G(u): u \in V(G)\}.$
On the contrary, let us assume that $D_G(v) > d_G(v), \forall v \in V(G).$
Then, $|d_G(v) - \Upsilon(G)| > d_G(v)$ and $d_G(v) - \Upsilon(G) > d_G(v).$

Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

Thus, $\Upsilon(G) < 0,$ which is a contradiction.
Therefore, $D_G(v) \le d_G(v) \Rightarrow D_G^2(v) \le d_G^2(v).$

$$\sum_{u,v \in E(G)} \sqrt{D_G^2(u) + D_G^2(v)} \le \sum_{u,v \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}$$
$$D_a SO(G) \le SO(G).$$

Theorem 2: If T is a full m-array tree with i internal vertices then,
$$D_a SO(T) = (i-1)|m-i|\sqrt{2} + [i(m-1)+1]\sqrt{m^2+1+2i^2-2i(m+1)}.$$

Proof: If T is a full m-array tree with I internal vertices then $p = mi + 1$ and $q = mi.$
All the internal vertices act as dominating vertices and hence $\Upsilon(G) = i.$ Since the degree of each internal vertex is m and the rest are pendant vertices, the dominational degree of i vertices is $|m-i|$ and the remaining $i(m-1) + 1$ vertices is $|1-i|.$
The edge partition is as follows:
$E_1 = \{D_G(u) = |m-i| = D_G(v)\}, |E_1| = (i-1),$
$E_2 = \{D_G(u) = |m-i|, D_G(v) = |1-i|\}, |E_2| = i(m-1) + 1.$
Thus, $D_a SO(T) = (i-1)|m-i|\sqrt{2} + [i(m-1)+1]\sqrt{m^2+1+2i^2-2i(m+1)}.$

Corollary: For a binary tree,
$$D_a SO(T) = (i-1)|2-i|\sqrt{2} + [i+1]\sqrt{5+2i^2-6i}.$$
Proof: A binary tree is a 2-full array tree, i.e., $m = 2.$
Hence the result.

3. Generalization of Dominational Variants of Sombor index for a family of standard graphs
Theorem 1: For a path graph $P_n (n \ge 3),$

a) $D_a SO(P_n) = 2\sqrt{2\Upsilon(G)^2 - 6\Upsilon(G) + 5} + (n-3)|1 - \Upsilon(G)|\sqrt{2}.$

b) $D_{HDR} SO(P_n) = \begin{cases} 2\sqrt{|1-\Upsilon(G)|^2 + |2-\Upsilon(G)|^2} + (n-3)|1-\Upsilon(G)|\sqrt{2}, & n \text{ is odd}, \\ (n-1)|1-\Upsilon(G)|\sqrt{2}, & n \text{ is even}. \end{cases}$

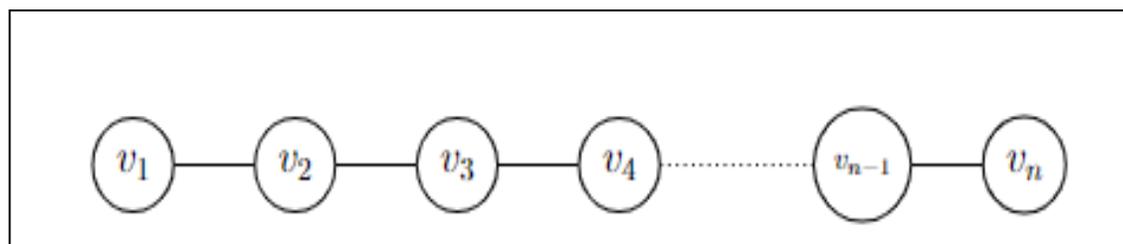**Figure 1:** Path graph

Proof a) A path graph is a connected acyclic graph with order $n,$ size $n-1$ and $\Upsilon(G) = \alpha = \left\lceil \frac{n}{3} \right\rceil.$
Based on the dominational degree, the edges can be classified as follows:
$E_1 = \{D_G(u) = |1-\alpha|, D_G(v) = |2-\alpha|\}, |E_1| = 2,$
$E_2 = \{D_G(u) = |1-\alpha| = D_G(v)\}, \qquad |E_2| = n - 3.$
Hence, $\qquad D_a SO(P_n) = 2\sqrt{2\alpha^2 - 6\alpha + 5} + (n-3)|1-\alpha|\sqrt{2}.$

Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

b) The eccentricities of the end vertices are full dgrees and decreases by one on either sides.

<u>Case i</u>: For odd n, the eccentricity of the $v_{\frac{n+1}{2}}$ vertex is $\frac{n-1}{2}$ and hence the radius is $\frac{n-1}{2}$.

The $d_{hr}(v_i) = 1$ and $D_{hr}(v_i) = |1 - \alpha|$ for all vertices except the central vertex $v_{\frac{n+1}{2}}$.

The edge partition is as follows:
$$E_1 = \{D_{hr}(u) = |1 - \alpha|, D_{hr}(v) = |2 - \alpha|\}, \quad |E_1| = 2,$$
$$E_2 = \{D_{hr}(u) = |1 - \alpha| = D_{hr}(v)\}, \qquad |E_2| = (n - 3).$$

Thus, the dominational HDR Somber Index is

$D_{HDR}SO(P_n) = 2\sqrt{|1 - \alpha|^2 + |2 - \alpha|^2} + (n - 3)|1 - \alpha|\sqrt{2}$ for odd 'n'.

<u>Case ii</u>: For even n, the eccentricity of the $v_{\frac{n}{2}}$ vertex is $\frac{n}{2}$ and hence the radius is $\frac{n}{2}$.

The $d_{hr}(v_i) = 1$ for all vertices except the central vertex $v_{\frac{n}{2}}$.

The edge partition is as follows:
$$E_1 = \{D_{hr}(u) = |1 - \alpha| = D_{hr}(v)\}, \quad |E_1| = (n - 1).$$

Thus, the dominational HDR Somber Index is

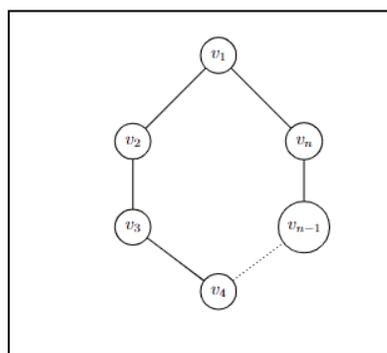$D_{HDR}SO(P_n) = (n - 1)|1 - \alpha|\sqrt{2}$ for even 'n'.

The dominational HDR Somber index for a path graph is

$$D_{HDR}SO(P_n) = \begin{cases} 2\sqrt{|1 - \alpha|^2 + |2 - \alpha|^2} + (n - 3)|1 - \alpha|\sqrt{2}, & n \text{ is odd,} \\ (n - 1)|1 - \alpha|\sqrt{2}, & n \text{ is even.} \end{cases}$$

Theorem 2: For a cycle graph C_n,

a) $D_d SO(C_n) = |2 - \alpha|\sqrt{2}n$, for $n \geq 7$.

b) $D_{HDR}SO(C_n) = \begin{cases} 2\sqrt{|1 - \alpha|^2 + |2 - \alpha|^2} + (n - 3)|1 - \alpha|\sqrt{2}, & n \text{ is odd,} \\ (n - 1)|1 - \alpha|\sqrt{2}, & n \text{ is even.} \end{cases}$

Proof: a) A cycle graph is a connected graph with $|V| = n$, $|E| = n$ and $\Upsilon(G) = \alpha = \left\lceil \frac{n}{3} \right\rceil$.

Based on the dominational degree, the edges can be classified as follows:
$$E_1 = \{D_G(u) = |2 - \alpha|, D_G(v) = |2 - \alpha|\}, \quad |E_1| = n.$$

Thus, $\qquad D_d SO(C_n) = |2 - \alpha|\sqrt{2}n$.

  b) The eccentricities of all the vertices is $\left\lceil \frac{n}{2} \right\rceil$.

<u>Case i</u>: For odd 'n', the $d_{hr}(v_i) = 2$ for all vertices.

The edge partition is as follows:
$$E_1 = \{D_{hr}(u) = |2 - \alpha| = D_{hr}(v)\}, \quad |E_1| = n.$$

Thus, the dominational HDR Somber Index is
$$D_{HDR}SO(C_n) = |2 - \alpha|n\sqrt{2} \text{ for odd 'n'.}$$

<u>Case ii</u>: For even 'n', the $d_{hr}(v_i) = 1$ for all vertices.

The edge partition is as follows:
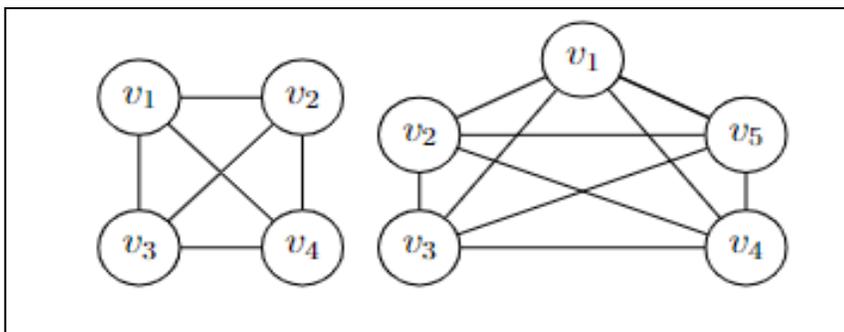$$E_1 = \{D_{hr}(u) = |1 - \alpha| = D_{hr}(v)\}, \quad |E_1| = n.$$

Thus, the dominational HDR Somber Index is
$D_{HDR}SO(C_n) = |1 - \alpha|n\sqrt{2}$ for even 'n'.

The dominational HDR Somber index for a cycle graph is
$$D_{HDR}SO(C_n) = \begin{cases} |2 - \alpha|n\sqrt{2}, & n \text{ is odd} \\ |1 - \alpha|n\sqrt{2}, & n \text{ is even.} \end{cases}$$

Theorem 3: For a complete graph K_n, $D_{HDR}SO(K_n) = D_d SO(K_n) = \frac{n(n-1)(n-2)}{\sqrt{2}}$.

Proof : A complete graph K_n is a connected (n-1) regular graph with 'n' vertices and $\frac{n}{2}C$ edges. Since in a complete graph, every vertex is adjacent to every other vertex eccentricity of every vertex is one and hence radius of a complete graph is 1. The domination number of a complete graph is unity.

The edge partition for the dominational degree is as follows:
$E_1 = \{D_G(u) = n - 2 = D_G(v)\}, |E_1| = \frac{n}{2}C.$

Thus, $D_d SO(K_n) = \frac{n(n-1)(n-2)}{\sqrt{2}}$.

Every vertex is a central vertex and hence $d_{hr}(v_i) = n - 1$.
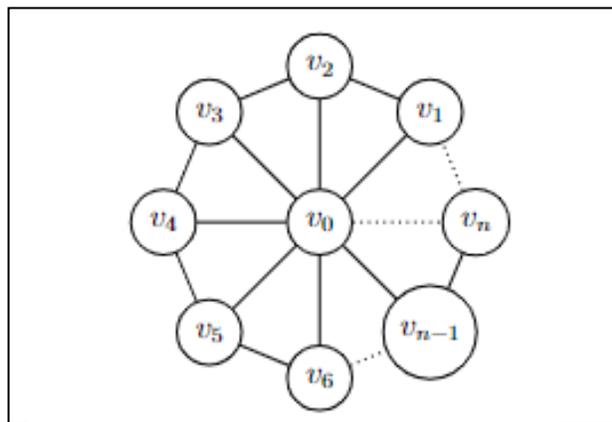
Hence the edge partition is
$$E_1 = \{D_{hr}(u) = D_{hr}(v) = |n - 2|\}, |E_1| = \frac{n(n-1)}{2}.$$

The dominational HDR Somber index is $D_{HDR}SO(K_n) = \frac{n(n-1)(n-2)}{\sqrt{2}}$.

Theorem 4: For a wheel graph $W_n (n \geq 4)$,

 a) $D_d SO(W_n) = (n - 1)\left[2\sqrt{2} + \sqrt{4 + (n - 2)^2}\right].$

 b) $D_{HDR}SO(W_n) = (n - 1)\left[\sqrt{8} + \sqrt{4 + (n - 2)^2}\right].$

Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

Proof: A wheel graph is a cyclic connected graph with n vertices, $2n - 2$ edges and $Y(G) = 1$.

A wheel graph $W_n = C_{n-1} + K_1$, where C_{n-1} is a cycle graph with n-1 vertices and K_1 is placed at the centre adjacent with all the n-1 vertices of the cycle.

    a) The edge partition for the dominational degree is as follows:

$$E_1 = \{D_G(u) = 2 = D_G(v)\}, \quad |E_1| = n - 1,$$
$$E_2 = \{D_G(u) = 2, D_G(v) = n - 2\}, \quad |E_2| = n - 1.$$

Thus, $$D_a SO(W_n) = (n - 1)\left[2\sqrt{2} + \sqrt{4 + (n - 2)^2}\right].$$

    b) The eccentricities of all the vertices belonging to the cycle is 3 and the eccentricity of the vertex of $K_{1\,is}\ n - 1$.

The edge partition is as follows:

$$E_1 = \{D_{hr}(u) = 2, D_{hr}(v) = 2\}, \ |E_1| = n - 1.$$
$$E_2 = \{D_{hr}(u) = 2, D_{hr}(v) = n - 2\}, \ |E_2| = n - 1.$$

Thus, $$D_{HDR} SO(W_n) = (n - 1)\left[\sqrt{8} + \sqrt{4 + (n - 2)^2}\right].$$

Theorem 5: For a friendship graph $F_n (n \geq 3)$, $D_{HDR} SO(F_n) = D_a SO(F_n)$.

Proof: A friendship graph is an cyclic connected graph with '2n+1' vertices and '3n' edges, obtained by placing 'n' copies of C_3 with a vertex in common.

The domination number of this graph is also found to be unity.

The edge partition for the dominational degree is as follows:

$E_1 = \{D_G(u) = 1, D_G(v) = 1\}, \quad |E_1| = n,$

$E_2 = \{D_G(u) = 1, D_G(v) = 2n - 1\}, \quad |E_2| = 2n.$

Thus, $D_a SO(F_n) = n\sqrt{2} + 2n\sqrt{(2n - 1)^2 + 1}$.

The eccentricity of the vertex in common to all the cycles is 1 and the eccentricity of all the other vertices is 2, which makes the radius of the graph to be 1.

The $d_{hr}(v_i) = 2$ for all vertices except the central vertex and for the central vertex

$d_{hr}(v) = 2n.$

The edge partition is as follows:

$$E_1 = \{D_{hr}(u) = 2n - 1, D_{hr}(v) = 1\}, \ |E_1| = 2n,$$
$$E_2 = \{D_{hr}(u) = 1, D_{hr}(v) = 1\}, \ |E_2| = n.$$

Thus, the HDR Somber Index is

$$D_{HDR}SO(F_n) = 2n\sqrt{4n(n-1) + 2}.$$

4. Determination of Dominational Status Sombor index for certain benzenoid hydrocarbons

Sl No.	Name	Dominational Status Sombor Index	Boiling Points
1	Napthalene	286.9397	218
2	Phenapthalene	766.81844	338
3	Anthracene	794.42712	340
4	Chrysene	2035.1254	431
5	Benz[a]anthracene	1741.3929	425
6	Triphenylene	1469.7624	429
7	Naphthacene	1695.0743	440
8	Benzo[c]pyrene	2053.6768	496
9	Benzo[e]pyrene	1952.5916	493
10	Perylene	1987.2752	497
11	Dibenzo[def.mno]chrysene	2584.6022	547
12	Benzo[ghi]perylene	2493.6565	542
13	Benzo[b]triphenylene	2704.7243	535
14	Dibenz[a,h]anthracene	2925.4312	536
15	Dibenzo[a,j]anthracene	2874.2855	531
16	Picene	2898.7559	519
17	Coronene	3207.169	590
18	Naphtho[1,2,3,4-def]chrysenre	3315.5145	592
19	Dibenzo[b.def]chrysenre	3545.6978	596
20	Benzo[rst]pentaphene	3527.6416	594
21	Dibenzo[def.p]chrysene	286.9397	595

Table 1: Determination of $D_\sigma(G)$

5. Results and Discussion

The dominational status Sombor and the boiling points of benzenoid hydrocarbons are connected via regression analysis. The plot and results are displayed below.
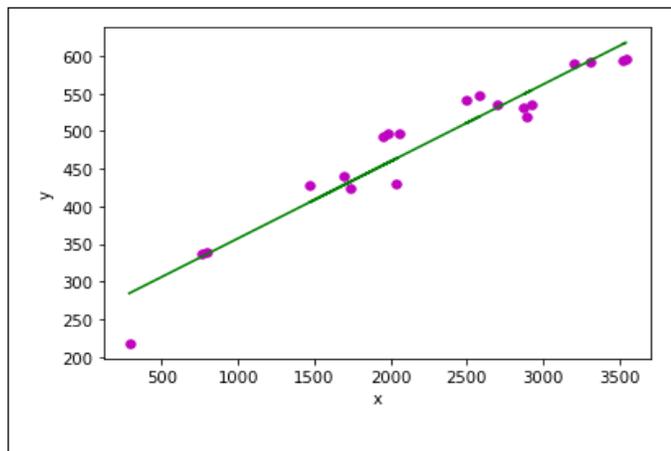
Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

Figure 5: Plot of Dominational Status Sombor index against Boiling points of Benzenoid hydrocarbons.

Using the linear regression, $BP = A[D_\sigma(G)] + B.$

The regression data for the above expression is as follows:

Multiple R	R Square	Intercept (B)	X Variable 1 (A)
0.96923	0.922042	255.1745	0.102217

The equation of the line of regression is given by:

$BP = 0.102217[D_\sigma(G)] + 255.1745.$

The regression co-efficient is found to be close to unity, implying that the Dominational Status Sombor can be used to determine boiling points.

6. Conclusion

Domination and topological index are two distinct fields of study in graph theory. An attempt was made to merge these two branches in order to identify appropriate applications of a molecular descriptor based on graph dominance. The dominational Status Sombor index is a good predictor of the boiling points of benzenoid hydrocarbons. The Status Connectivity index[4] produced the best results, with R=0.968. This confirms that the outcome is justifiable.

References

1. Gutman, Geometric approach to degree-based topological indices: Sombor Indices,MATCH Communications in Mathematical and Computer Chemistry 86, (2021).
2. 11-16.
3. V. R. Kulli, HDR Nirmala index, International Journal of Mathematics and Computer Research 10 (2022), 2796-2800.DOI: https://doi.org/10.47191/ijmcr/v10i7.03.
4. V. R. Kulli, HDR Somber Indices and Their Exponentials of a Graph, International Journal of
5. Mathematics and Computer Research 10 (2022), 2814-2821.DOI: https://doi.org /10.47191 /ijmcr/v10i7. 07.

6. H.S. Ramane, and A.S. Yalnaik, Status connectivity indices of graphs and its applications to the boiling point of benzenoid hydrocarbons. Journal of Applied Mathematics and Computing, 55(1) (2016), 609-662.DOI:https://doi.org/10.1007/s12190-016-1052-5.

7. V. R. Kulli, Status Sombor indices, International Journal of Mathematics and Computer Research, 10 (2022), 2726-2730.DOI: https://doi.org/10.47191/ijmcr/v10i6.05.

8. S. Hegde, G. Sharma, and R. Hegde, Sombor index of certain standard graphs, In AIP Conference

9. Proceedings, AIP Publishing LLC, 2516(1) (2022).DOI: https://doi.org/10.1063/5.0108773.

10. S. Hosamani, D. Perigidad, S. Jamagoud, Y. Maled, and S. Gavade, QSPR analysis of certain degree based topological indices, Journal of Statistics Applications & Probability, 6(2) (2017),361-371.

11. R. G. Domenech, J. Gálvez, J. V. de Julián-Ortiz, and L. Pogliani, Some new trends in chemical

12. Graph theory. Chemical Reviews, 108(3) (2008), 1127-1169.

13. K. C. Das, K. Xu, J. Nam, Zagreb indices of graphs, Frontiers of Mathematics in China, 10(3)(2015), 567-582.

14. S. Gupta, M. Singh, A. K. Madan, Application of graph theory: Relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity. Journal of Mathematical Analysis and Applications, 266(2) (2002), 259-268.

15. S. Gupta, M. Singh, and A.K. Madan, Applications of graph theory: Relationship of molecular

16. Connectivity index and atomic molecular connectivity index with anti-HSV activity. Journal of

17. Molecular Structure: THEOCHEM, 571(1-3) (2001), 147-152.