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NEIGHBOR SOMBOR INDEX: MATHEMATICAL PROPERTIES AND ITS CHEMICAL APPLICABILITIES

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ABSTRACT. Gutman introduced the so-called Sombor index, a unique degree-based graphical index having geometrical importance. In a similar manner, Kulli extended the neighborhood version of the Sombor index for the graph G. In this paper, several bounds and characterizations are obtained. Along with the chemical application in nitro polycyclic aromatic hydrocarbons (nitro-PAHs), several relationships between the neighbor Sombor index and other degree and neighbor sum based graphical indices are also obtained.

1. Introduction

All the graphs $G = (V, E)$ considered here are simple, finite, non-trivial and undirected, where $\mid V \mid= n$ denotes the number of vertices and $\mid E \mid= m$ denotes the number of edges of G. The degree d_v of a vertex v is the number of vertices adjacent to v. The minimum degree and maximum degree are represented by $\delta = \delta(G)$ and $\Delta = \Delta(G)$ respectively. The set of all vertices which are adjacent to a vertex v is called open neighborhood of v and denoted by $N(v)$. The closed neighborhood of a vertex v is the set $N[v] = N(v) \cup \{v\}$. For graph theoretical terminology and notation not defined here, we follow [**12**].

A molecular graph is a graph where the edges represent bonds in a molecule and the vertices represent atoms. A graphical index [**26**] is a single number that may be calculated from the molecular graph and used to describe a particular attribute of the underlying molecule. Recently, Gutman [**8**] introduced a novel

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degree-based topological index, called the Sombor index. It was inspired by the geometric interpretation of degree-radii of the edges and is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}. \tag{1.1}$$

Since then, many graph theorists showed interest in finding some potential mathematical properties and their chemical applicabilities of this novel degree based index along with geometrical significance. For instance, we refer to [**3, 4, 5, 9, 15, 14, 16, 22, 24, 27**]. Also, many neighbor sum related indices and parameters were also introduced. See [**2, 13, 19, 20, 21**]. Analogously, Kulli [**13**] introduced the neighborhood Sombor (or simply, neighbor Sombor) index of a graph G which is defined as

$$NS(G) = \sum_{uv \in E(G)} \sqrt{S_u^2 + S_v^2}. \tag{1.2}$$

where S_x is the degree sum of neighbor vertices of x in $V(G)$ (i.e., $S_x = \sum_{y \in N(x)} d_y$).

In this paper, the first part contains the bounds and characterization and second part contains the chemical applicability of neighbor Sombor index.

2. Mathematical inequalities

2.1. Inequality in terms of order and size. Let G be a non-trivial (n, m)-graph. Note that for each $uv \in E(G)$,

$$1 \leqslant \{S_u, S_v\} \leqslant (n-1)^2. \tag{2.1}$$

From equations (1.2) and (2.1), we have for each $uv \in E(G)$, the sum S_u^2 and S_v^2 gives $2 \leqslant S_u^2 + S_v^2 \leqslant 2(n-1)^4$. Summing up this inequality over the edges $uv \in E(G)$, we get the inequality of $NS(G)$ in terms of order and size as,

$$\sqrt{2}\, m \leqslant NS(G) \leqslant \sqrt{2}\, m\, (n-1)^2. \tag{2.2}$$

2.2. Inequality in terms of size and minimum / maximum degree. Let G be a non-trivial connected (n, m)-graph. Note that for the vertices $u, v \in V(G)$,

$$\delta(G)^2 \leqslant \{S_u, S_v\} \leqslant \Delta(G)^2. \tag{2.3}$$

From equations (1.2) and (2.3), we have for each $uv \in E(G)$, the sum S_u^2 and S_v^2 gives $2\delta(G)^4 \leqslant S_u^2 + S_v^2 \leqslant 2\Delta(G)^4$. Summing up this inequality over the edges $uv \in E(G)$, we get the inequality of $NS(G)$ in terms of size and minimum / maximum degree as,

$$\sqrt{2}\, m\, \delta(G)^2 \leqslant NS(G) \leqslant \sqrt{2}\, m\, \Delta(G)^2. \tag{2.4}$$

Further, equation (2.4) is attained if and only if G is a regular graph.

For example, $NS(C_n) = 4\sqrt{2}n$ and $NS(K_n) = \dfrac{n(n-1)^3}{\sqrt{2}}$, where C_n; $n \geqslant 3$ is a cycle and K_n is a complete graph.

2.3. Inequality in terms of size and minimum / maximum neighborhood degree sum.

LEMMA 2.1. [**18**] *Let G be a non-trivial connected (n, m)-graph with $\Delta_N(G) = max\{S_u : u \in V(G)\}$ and $\delta_N(G) = min\{S_u : u \in V(G)\}$. Then $\delta_N(G) \leqslant \{S_u\} \leqslant \Delta_N(G)$ for all $u \in V(G)$. Further, the equality holds if and only if G is a regular graph or a complete bipartite graph.*

Let G be a non-trivial connected graph. By Lemma (2.1), we have

$$\delta_N(G) \leqslant \{S_u, S_v\} \leqslant \Delta_N(G) \text{ for all } u, v \in V(G). \tag{2.5}$$

Summing up this inequality (2.5) over the edges $uv \in E(G)$, we get the inequality of $NS(G)$ in terms of size and minimum / maximum neighborhood degree sum as,

$$\sqrt{2}\, m\, \delta_N(G) \leqslant NS(G) \leqslant \sqrt{2}\, m\, \Delta_N(G). \tag{2.6}$$

Further, the equality holds if and only if G is a regular graph or a complete bipartite graph.

2.4. Inequality in terms of Sombor index. Let G be a non-trivial (n, m)-graph. Note that for each $uv \in E(G)$,

$$d_u \leqslant S_u \leqslant \Delta(G)d_u \text{ and } d_v \leqslant S_v \leqslant \Delta(G)d_v. \tag{2.7}$$

From equations (1.1), (1.2) and (2.7), we have an inequality of $NS(G)$ in terms of Sombor index as,

$$SO(G) \leqslant NS(G) \leqslant \Delta(G)SO(G). \tag{2.8}$$

2.5. Inequalities in terms of Zagreb indices. The first Zagreb and second Zagreb indices were introduced by Gutman et al. in [**11**] and [**10**] respectively. The first and the second Zagreb indices of a graph G are defined as

$$M_1(G) = \sum_{uv \in E(G)} [d_u + d_v] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} [d_u d_v].$$

LEMMA 2.2. [**1**] *For any non-trivial (n, m)-graph G,*

$$\sum_{v \in V(G)} S_v = M_1(G).$$

To prove our next result, we make use of the relations between Sombor index and Zagreb indices, which are studied by [**4**], [**5**] and [**16**] that are as follows.

LEMMA 2.3. *For any non-trivial (n, m)-graph G,*

(i) $\frac{1}{\sqrt{2}} M_1(G) \leqslant SO(G) \leqslant M_1(G)$.

(ii) $\frac{\sqrt{2}}{n-1} M_2(G) \leqslant SO(G) \leqslant \sqrt{\left(\frac{\Delta(G)}{\delta(G)} + \frac{\delta(G)}{\Delta(G)}\right) m M_2(G)}$.

Let G be a non-trivial (n,m)-graph. By equation (2.8) and Lemma 2.3, we have the inequalities of $NS(G)$ in terms of Zagreb indices as,

$$\frac{1}{\sqrt{2}}\, M_1(G) \leqslant NS(G) \leqslant \Delta(G)\, M_1(G). \tag{2.9}$$

$$\frac{\sqrt{2}}{n-1}\, M_2(G) \leqslant NS(G) \leqslant \Delta(G)\sqrt{\left[\frac{\Delta(G)}{\delta(G)} + \frac{\delta(G)}{\Delta(G)}\right] m\, M_2(G)}. \tag{2.10}$$

2.6. Inequalities in terms of Forgotten index. Followed by the Zagreb indices, the Forgotten index was defined in 1972 in [**11**]. This was later investigated by Furtula and Gutman in 2015 in [**6**] which is defined as

$$F(G) = \sum_{uv\in E(G)} [d_u^2 + d_v^2].$$

LEMMA 2.4. [**6**] *For any non-trivial (n,m)-graph G,*

$$\frac{M_1(G)^2}{m} - 2M_2(G) \leqslant F(G) \leqslant 2M_2(G) + m(n-2).$$

Let G be a non-trivial graph. By equations (1.2) and (2.7), we have

$$\begin{aligned} NS(G) = \sum_{uv\in E(G)} \sqrt{S_u^2 + S_v^2} &= \sum_{uv\in E(G)} \left[\frac{S_u}{S_v} + \frac{S_v}{S_u}\right] \sqrt{\frac{1}{\frac{1}{S_u^2} + \frac{1}{S_v^2}}} \\ &\leqslant \sum_{uv\in E(G)} \left[\frac{\Delta d_u}{d_v} + \frac{d_v}{\Delta d_u}\right] \sqrt{\frac{1}{\frac{1}{\Delta^2 d_u^2} + \frac{1}{\Delta^2 d_v^2}}} \\ &\leqslant \sum_{uv\in E(G)} \Delta \left[\frac{d_u}{d_v} + \frac{d_v}{d_u}\right] \Delta \sqrt{\frac{1}{\frac{1}{d_u^2} + \frac{1}{d_v^2}}} = \frac{\Delta^3}{\sqrt{2}\delta^2} F(G). \end{aligned}$$

Similarly,

$$\begin{aligned} \sum_{uv\in E(G)} \left[\frac{\Delta d_u}{d_v} + \frac{d_v}{\Delta d_u}\right] \sqrt{\frac{1}{\frac{1}{\Delta^2 d_u^2} + \frac{1}{\Delta^2 d_v^2}}} &\geqslant \sum_{uv\in E(G)} \left[\frac{d_u}{d_v} + \frac{d_v}{d_u}\right] \sqrt{\frac{1}{\frac{1}{d_u^2} + \frac{1}{d_v^2}}} \\ &= \frac{\delta}{\sqrt{2}\Delta^2} F(G). \end{aligned}$$

Thus we have an inequality of $NS(G)$ in terms of Forgotten index as,

$$\frac{\delta}{\sqrt{2}\Delta^2} F(G) \leqslant NS(G) \leqslant \frac{\Delta^3}{\sqrt{2}\delta^2} F(G). \tag{2.11}$$

Also, from Lemma 2.4 and equation (2.11), we have,

$$\frac{\delta}{\sqrt{2}\Delta^2}\left[\frac{M_1(G)^2}{m} - 2M_2(G)\right] \leqslant NS(G) \leqslant \frac{\Delta^3}{\sqrt{2}\delta^2}\left[2M_2(G) + m(n-2)\right].$$

2.7. Inequalities in terms of Randic index. In 1975, the chemist Milan Randic proposed a topological index under the name branching index [**23**], later this was know as Randic index and defined as

$$R(G) = \frac{1}{\sqrt{d_u.d_v}}.$$

(i) Let G be a non-trivial graph. By equations (1.2),(2.3) and (2.7), we have

$$NS(G) = \sum_{uv\in E(G)} \sqrt{S_u^2 + S_v^2} = \sum_{uv\in E(G)} \frac{1}{\sqrt{S_u.S_v}} \sqrt{S_u S_v \left[S_u^2 + S_v^2\right]}$$

$$\leqslant \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u.d_v}} \sqrt{\Delta^2\Delta^2\left[\Delta^4 + \Delta^4\right]} = \sqrt{2}\Delta^4 R(G).$$

Similarly, $NS(G) \geqslant \dfrac{\sqrt{2}\delta^4}{\Delta} R(G)$.

Therefore, the inequality of $NS(G)$ in terms of Randic index is,

$$\frac{\sqrt{2}\delta^4}{\Delta} R(G) \leqslant NS(G) \leqslant \sqrt{2}\Delta^4 R(G). \tag{2.12}$$

(ii) Let G be a non-trivial graph. By equations (1.2),(2.3) and (2.7), we have,

$$\frac{\sqrt{2}}{n-1} R(G) \leqslant NS(G) \leqslant (n-1)^3 R(G). \tag{2.13}$$

2.8. Inequalities in terms of hyper Zagreb indices. Shirdel et al. [**25**] introduced the hyper Zagreb indices which are defined as,

$$HM_1(G) = \sum_{uv\in E(G)} (d_u + d_v)^2 \quad \text{and} \quad HM_2(G) = \sum_{uv\in E(G)} (d_u.d_v)^2.$$

Lemma 2.5. [**27**] *For any connected graph G,*

$$\frac{HM_1(G)}{2\sqrt{2}\Delta} \leqslant SO(G) \leqslant \frac{HM_1(G)}{2\delta} - \frac{\delta m}{2} - \frac{\delta^2 m}{2\sqrt{8\Delta^2 + \delta^2} + 4\sqrt{2}\Delta}$$

(i) Let G be a connected graph. By equations (1.2), (2.8) and lemma 2.5, we have an inequality of $NS(G)$ in terms of the first Hyper Zagreb index as,

$$\frac{HM_1(G)}{2\sqrt{2}\Delta} \leqslant NS(G) \leqslant \Delta\frac{HM_1(G)}{2\delta} - \frac{\delta m}{2} - \frac{\delta^2 m}{2\sqrt{8\Delta^2 + \delta^2} + 4\sqrt{2}\Delta} \tag{2.14}$$

(ii) Let G be a non-trivial graph. By equations (1.2), (2.3) and (2.7), we have,

$$NS(G) = \sum_{uv\in E(G)} \sqrt{S_u^2 + S_v^2} = \sum_{uv\in E(G)} S_u^2 + S_v^2 \sqrt{\left(\frac{1}{S_u^2 S_v^4} + \frac{1}{S_u^4 S_v^2}\right)}$$

$$\leqslant \sum_{uv\in E(G)} \Delta^4 d_u^2 + d_v^2 \frac{\sqrt{2}}{\delta^3} = \sqrt{2}\frac{\Delta^4}{\delta^3} HM_2(G).$$

Similarly, $NS(G) \geqslant \dfrac{\sqrt{2}}{\Delta^3} HM_2(G)$.

Thus, we have an inequality of $NS(G)$ in terms of the second Hyper Zagreb index as,

$$\frac{\sqrt{2}}{\Delta^3}HM_2(G) \leqslant NS(G) \leqslant \sqrt{2}\frac{\Delta^4}{\delta^3}HM_2(G). \tag{2.15}$$

2.9. Inequalities in terms of neighbor Zagreb indices. Graovac et al.[**7**] introduced the fifth M_1 and M_2 Zagreb indices which are based on neighbor degree sum that are defined as,

$$NM_1(G) = \sum_{uv\in E(G)} [S_u + S_v] \quad \text{and} \quad NM_2(G) = \sum_{uv\in E(G)} [S_u S_v].$$

(i) Let G be a non-trivial graph. By equations (1.2) and (2.7), we have,

$$\begin{aligned} NS(G) &= \sum_{uv\in E(G)} \sqrt{S_u^2 + S_v^2} = \sum_{uv\in E(G)} \sqrt{(S_u + S_v)^2 - 2S_uS_v} \\ &\geqslant \sum_{uv\in E(G)} \left[\sqrt{(S_u + S_v)^2} - \sqrt{2S_uS_v}\right] \\ &\geqslant NM_1(G) - \sqrt{2}\Delta^2. \end{aligned}$$

Thus we have an inequality of $NS(G)$ in terms of the fifth M_1 Zagreb index as,

$$NM_1(G) - \sqrt{2}\Delta^2 \leqslant NS(G). \tag{2.16}$$

(ii) Let G be a non-trivial graph. By equations (1.2) and (2.7), we have,

$$\begin{aligned} NS(G) &= \sum_{uv\in E(G)} \sqrt{S_u^2 + S_v^2} \\ &= \sum_{uv\in E(G)} S_uS_v\sqrt{\frac{1}{s_u^2} + \frac{1}{s_v^2}} \\ &\leqslant \frac{\sqrt{2}}{\delta}NM_2(G). \end{aligned}$$

Similarly, $NS(G) \geqslant \dfrac{\sqrt{2}}{\Delta\sqrt{\Delta}}NM_2(G)$.

Thus we have an inequality of $NS(G)$ in terms of the fifth M_2 Zagreb index as,

$$\frac{\sqrt{2}}{\Delta\sqrt{\Delta}}NM_2(G) \leqslant NS(G) \leqslant \frac{\sqrt{2}}{\delta}NM_2(G). \tag{2.17}$$

2.10. Inequalities in terms of first and fourth NDe indices. Sourav Mondal et al. [**18**] introduced first NDe index (ND_1) and fourth NDe index (ND_4) which are defined as

$$ND_1(G) = \sum_{uv\in E(G)} \sqrt{S_u.S_v} \quad \text{and} \quad ND_4(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{S_u.S_v}}.$$

(i) Let G be a non-trivial graph. By equations (1.2) and (2.3), we have,

$$NS(G) = \sum_{uv \in E(G)} \sqrt{S_u^2 + S_v^2} = \sum_{uv \in E(G)} \sqrt{S_u S_v \left(\frac{S_u}{S_v} + \frac{S_v}{S_u} \right)}$$
$$\leqslant ND_1(G) \sqrt{\left(\frac{S_u}{S_v} + \frac{S_v}{S_u} \right)}.$$

Also,

$$NS(G) = \sum_{uv \in E(G)} \sqrt{S_u^2 + S_v^2}$$
$$\geqslant \sum_{uv \in E(G)} \sqrt{2 S_u S_v} = \sqrt{2} ND_1(G).$$

Thus, we have an inequality of $NS(G)$ in terms of first NDe index as,

$$\sqrt{2} ND_1(G) \leqslant NS(G) \leqslant ND_1(G) \sqrt{\left(\frac{S_u}{S_v} + \frac{S_v}{S_u} \right)} \tag{2.18}$$

(ii) Let G be a non-trivial graph. By equations (1.2) and (2.3), we have,

$$NS(G) = \sum_{uv \in E(G)} \sqrt{S_u^2 + S_v^2}$$
$$= \sum_{uv \in E(G)} \frac{1}{\sqrt{S_u S_v}} \sqrt{S_u S_v \left[S_u^2 + S_v^2 \right]}$$
$$\leqslant \sqrt{2} \Delta^3 ND_4(G)$$

Thus, we have an inequality of $NS(G)$ in terms of fourth NDe index as,

$$\sqrt{2} \delta^3 ND_4(G) \leqslant NS(G) \leqslant \sqrt{2} \Delta^3 ND_4(G). \tag{2.19}$$

Further equality holds iff G is regular.

3. Chemical applicabilities of neighbor Sombor index with niro-PAHs

The nitro-polycyclic aromatic hydrocarbons (nitro-PAHs) are a type of polycyclic aromatic hydrocarbons that has one or more nitro substituents added to it. These have been identified as a class of chemicals that have been detected in a variety of environmental sources and their presence in cigarette smoke has also been suggested. The nitro-PAHs can be generated in the environment through combustion or atmospheric interactions of PAHs and nitrogen oxides, both of which are common environmental pollutants. These have been proven to have a wide range of biological functions. Recent research has discovered that atmospheric transformations are a major source of nitro-PAHs in the atmosphere.

We have considered unicyclic nitro-PAHs (one-benzo-ring nitroarenes) for our study. We here have calculated the different varities of Graphical indices along with the neighbor Sombor index and have compared the values of all nitro-PAHs using the graph. Table(1) represents the degree and neighborhood bond partitions of 15 hydrogen and oxygen suppressed unicyclic nitro-PAHs where (d_u, d_v) and (n_u, n_v) represents the vertex degree pair and vertex neighbor sum pair of an edge and k represents the cardinality of such partitions. Table(2) represents the calculated Graphical indices values of nitro-PAHs.

nitro-PAHs	Degree and neighbor degree sum bond partition and their cardinalities						
$1,3-Dinitrobenzene(nP_1)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)			
	k	2	2	4			
	(S_u, S_v)	(3,5)	(4,5)	(5,5)	(5,6)		
	k	2	2	2	2		
$1,3,5-Trinitrobenzene(nP_2)$	(d_u, d_v)	(1,3)	(2,3)				
	k	3	6				
	(S_u, S_v)	(3,5)	(5,6)				
	k	3	6				
$4-Nitrotoulene(nP_3)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)			
	k	2	2	4			
	(S_u, S_v)	(3,5)	(5,5)				
	k	2	6				
$2,3-Dinitrotoulene(nP_4)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	3	2	2	2		
	(S_u, S_v)	(3,6)	(3,7)	(4,5)	(5,6)	(6,7)	
	k	2	1	2	2	2	
$2,4-Dinitrotoulene(nP_5)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	3	1	4	1		
	(S_u, S_v)	(3,5)	(3,6)	(5,5)	(5,6)	(6,6)	
	k	1	2	2	2	2	
$2,5-Dinitrotoulene(nP_6)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	3	1	4	1		
	(S_u, S_v)	(3,5)	(3,6)	(5,5)	(5,6)	(6,6)	
	k	1	2	2	2	2	
$2,6-Dinitrotoulene(nP_7)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	3	2	2	2		
	(S_u, S_v)	(3,6)	(3,7)	(4,5)	(5,6)	(6,7)	
	k	2	1	2	2	2	
$3,4-Dinitrotoulene(nP_8)$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	3	1	4	1		
	(S_u, S_v)	(3,5)	(3,6)	(5,5)	(5,6)	(6,6)	
	k	1	2	2	2	2	
$3,5-Dinitrotoulene(nP_9)$	(d_u, d_v)	(1,3)	(2,3)				
	k	3	6				
	(S_u, S_v)	(3,5)	(5,6)				
	k	3	6				
$2,3,4-Trinitrotoulene(nP_{10})$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	4	1	2	3		
	(S_u, S_v)	(3,6)	(3,7)	(5,5)	(5,6)	(6,7)	(7,7)
	k	2	2	1	2	2	1
$2,3,5-Trinitrotoulene(nP_{11})$	(d_u, d_v)	(1,3)	(2,3)	(3,3)			
	k	4	4	2			
	(S_u, S_v)	(3,5)	(3,6)	(3,7)	(5,6)	(6,6)	(6,7)
	k	1	2	1	2	2	2
$2,3,6-Trinitrotoulene(nP_{12})$	(d_u, d_v)	(1,3)	(2,2)	(2,3)	(3,3)		
	k	4	1	2	3		
	(S_u, S_v)	(3,6)	(3,7)	(5,5)	(5,6)	(6,7)	(7,7)
	k	2	2	1	2	2	1
$2,4,5-Trinitrotoulene(nP_{13})$	(d_u, d_v)	(1,3)	(2,3)	(3,3)			
	k	4	4	2			
	(S_u, S_v)	(3,6)	(6,6)				
	k	4	6				
$2,4,6-Trinitrotoulene(nP_{14})$	(d_u, d_v)	(1,3)	(2,3)	(3,3)			
	k	4	4	2			
	(S_u, S_v)	(3,5)	(3,6)	(3,7)	(5,6)	(6,6)	(6,7)
	k	1	2	1	2	2	2
$3,4,5-Trinitrotoulene(nP_{15})$	(d_u, d_v)	(1,3)	(2,3)	(3,3)			
	k	4	4	2			
	(S_u, S_v)	(3,5)	(3,6)	(3,7)	(5,6)	(6,6)	(6,7)
	k	1	2	1	2	2	2

TABLE 1. Bond partitions of nitro-PAHs

Sl.No	nitro-PAHs	M_1	M_2	HM_1	HM_2	F	R	SO	NS	NM_1	NM_2	ND_1	ND_4
1	nP_1	36	38	164	194	88	3.7877	26.4036	54.2308	76	180	37.6447	1.7288
2	nP_2	42	45	198	243	108	4.1815	31.1201	64.3543	90	225	44.4823	1.87
3	nP_3	36	38	164	194	88	3.7877	26.4036	54.0883	76	180	37.746	1.7164
4	nP_4	42	47	202	293	108	4.2152	30.8401	67.898	94	241	45.9281	1.8106
5	nP_5	42	46	200	268	108	4.1984	30.9801	65.9806	92	233	45.3127	1.8281
6	nP_6	42	46	200	268	108	4.1984	30.9801	65.9806	92	233	45.3127	1.8281
7	nP_7	42	47	202	293	108	4.2152	30.8401	67.898	94	241	45.9281	1.8106
8	nP_8	42	46	200	268	108	4.1984	30.9801	65.9806	92	233	45.3127	1.8281
9	nP_9	42	45	198	243	108	4.1815	31.1201	64.3543	90	225	44.4823	1.87
10	nP_{10}	48	55	238	367	128	4.6259	35.4166	79.6781	110	296	53.5664	1.9245
11	nP_{11}	48	54	236	342	128	4.6091	35.5566	77.8933	108	288	52.8568	1.955
12	nP_{12}	48	55	238	367	128	4.6259	35.4166	79.6781	110	296	53.5664	1.9245
13	nP_{13}	48	54	236	342	128	4.6091	35.5566	77.7445	108	288	52.9706	1.9428
14	nP_{14}	48	54	236	342	128	4.6091	35.5566	77.8933	108	288	52.8568	1.955
15	nP_{15}	48	54	236	342	128	4.6091	35.5566	77.8933	108	288	52.8568	1.955

Table 2. Graphical indices of nitro-PAHs

4. Comparative analysis

All the graphical indices calculated using the molecular graphs of nitro-PAHs have been plotted and is represented by Figure 1. It is very clear from the figure that all the indices exhibit same pattern of graph. That is, if one of the indices values is low/high for a compound, then the other index values are also low/high respectively for that compound. Neighbor Sombor index lies between significantly proven topological indices. Hence it has a good significance. Neighbor Sombor index lies nearly between second Zagreb and neighbor first Zagreb indices. The first ND_e index and the second Zagreb indices are too close to each other where their difference is very small. Similarly Randic and fourth ND_e indices also have small difference. The second Hyper Zagreb index values are very high and the fourth ND_e index values are very low. In short, the comparison can be mathematically represented as,

$$ND_4(G) \leqslant R(G) \leqslant SO(G) \leqslant M_1(G) \leqslant ND_1(G) \leqslant M_2(G)$$
$$\leqslant NS(G) \leqslant NM_1(G) \leqslant F(G) \leqslant HM_1(G) \leqslant NM_2(G) \leqslant HM_2(G)$$

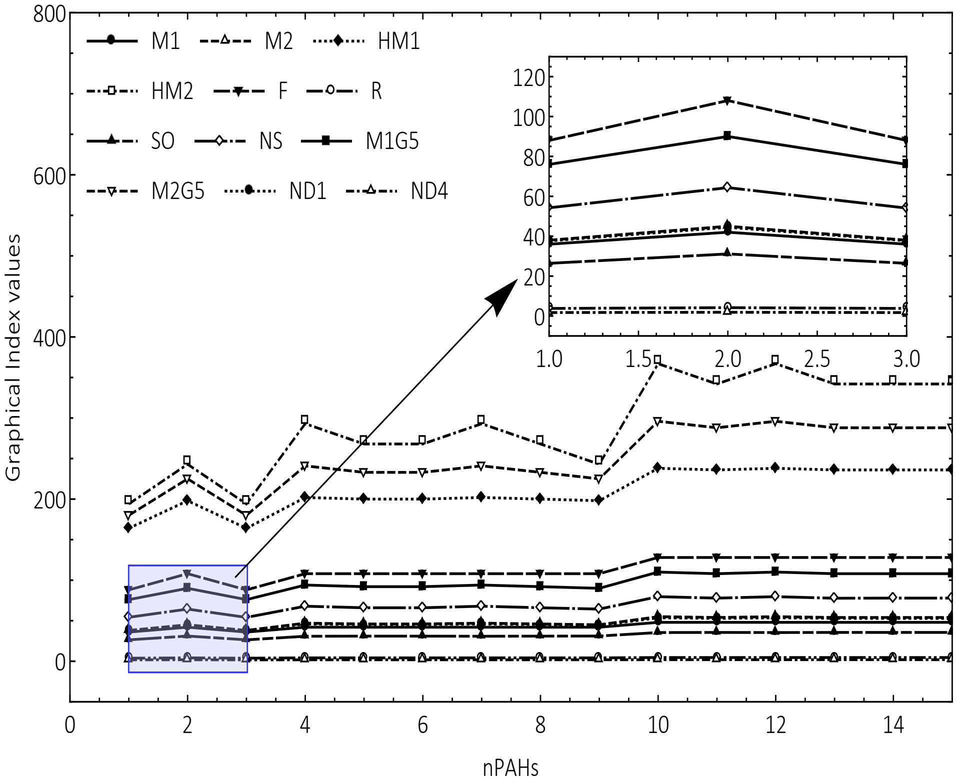

FIGURE 1. Graphical indices comparison

5. Conclusion and open problems

In this paper, we have discussed some bounds and characterizations on the neighbor Sombor index in terms of order and size, minimum / maximum vertex degree, minimum / maximum neighbor sum and the other few graphical indices. This index is an extension of a well established degree based index in terms of neighbor sum. Also, the comparative analysis of Graphical indices is made possible by computing the various graphical indices of molecular graphs connected with chemical graphs of nitro-PAHs.

Open problems: Since the graphical index in terms of neighbor degree (valency) sum like the neighborhood Sombor index of a (Chemical) graph is newly initiated, the mathematical properties, comparative advantages and applications are relatively unknown. For these reasons, many questions are suggested by this research, among them are the following.

(1) QSPR / QSAR analysis of these nitro-PAHs can be carried out to see how well the neighbor Sombor index is correlated with other indices calculated.

(2) Try to figure out which particular chemical property does this index represent.

(3) Try to generalize the neighbor Sombor related indices such as the generalized Neighbor index ($N_{(a,b)}(G)$), the generalized Non-neighbor index ($NN_{(a,b)}(G)$) and the generalized Neighbor coindex ($\overline{N}_{(a,b)}(G)$) which can be defined as

(a) $N_{(a,b)}(G) = \sum_{uv \in E(G)} \left[S_G(u)^a + S_G(v)^a\right]^b$;

(b) $NN_{(a,b)}(G) = \sum_{uv \in E(G)} \left[\overline{S_G(u)}^a + \overline{S_G(v)}^a\right]^b$;

(c) $\overline{N}_{(a,b)}(G) = \sum_{uv \notin E(G)} \left[S_G(u)^a + S_G(v)^a\right]^b$,

where a,b are integers, $S_G(x) = \sum_{y \in N(x)} d_y$ and $\overline{S_G(x)} = \sum_{y \notin N[x]} d_y$. Here, the neighbor Sombor index $N_{(2,\frac{1}{2})}(G)$, the Non-neighbor Sombor index $NN_{(2,\frac{1}{2})}(G)$ and the neighbor Sombor co-index $\overline{N}_{(2,\frac{1}{2})}(G)$.

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