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BASAVA AND HYPER-BASAVA INDICES OF GRAPHS

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Abstract: Inspired by the recent work of the Gourava and hyper-Gourava indices, we propose a new topological indices, the Basava and hyper-Basava indices of a molecular graph. Further, we compute the Basava and hyper-Basava indices of some standard class of graphs. The Basava and hyper-Basava indices are tested with physico-chemical properties of octane isomers such as entropy, acentric factor and DHVAP using linear regression models. The first Basava index highly correlates with acentric factor (coefficient of correlation **0.9590748**) and the second Basava index highly correlates with entropy (coefficient of correlation **0.9491009**). Finally, we compute the Basava and hyper-Basava indices of certain families of nanostar dendrimers. The obtained results can be used in data mining, particularly in researching the uniqueness of hyper-branched molecular graphs.

Keywords and Phrases: Basava indices, hyper-Basava indices, octane isomers, dendrimers.

2020 Mathematics Subject Classification: 05C09, 05C92.

1. Introduction and Preliminaries

Chemical graph theory is a branch of the mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that

can be used to characterize some property of the graph of a molecular structure is called a topological index for that graph. The topological indices play vital role in mathematical chemistry, especially quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) investigations. For chemical applications of topological indices refer [6, 7, 9, 10, 18, 19, 20, 21, 22].

In recent years, the application of dendrimers in biomedicine attracted much attention from researchers. Dendrimers are a class of well defined hyperbranched polymers. Dendrimers are used as a tool for drug discovery, cell repair, tissue regenerators, MRI contrast agents and anticancer drug carriers. For more details about dendrimers refer to [14].

In this paper, we are concerned with simple graphs, having no directed or weighted edges and no loops. Let G be a finite graph with n vertices and m edges is called (n, m) graph. We denote vertex set and edge set of graph G as $V(G)$ and $E(G)$, respectively. The *neighbourhood* of a vertex $u \in V(G)$ is defined as the set $N_G(u)$ consisting of all vertices v which are adjacent to u in G. The degree of a vertex $d_G(v)$ is the number of edges incident to it in G. Let $S_G(v) = \sum_{u \in N_G(v)} d_G(u)$ be the degree sum of neighbour vertices. For undefined graph theoretic terminologies and notations refer [8].

Graovac et al. [5] defined fifth M-Zagreb indices as

$$M_1G_5(G) = \sum_{v \in V(G)} \Big(S_G(u) + S_G(v)\Big),$$

and

$$M_2G_5(G) = \sum_{uv \in E(G)} S_G(u) \cdot S_G(v).$$

In [11], Kulli defined fifth hyper M-Zagreb indices as

$$HM_1G_5(G) = \sum_{v \in V(G)} \Big(S_G(u) + S_G(v)\Big)^2,$$

and

$$HM_2G_5(G) = \sum_{uv \in E(G)} (S_G(u) \cdot S_G(v))^2.$$

Kulli introduced the first Gourava index and second Gourava index of a molecular graph [12] as follows:

$$GO_1(G) = \sum_{uv \in E(G)} \big[d_G(u) + d_G(v) + d_G(u)d_G(v)\big],$$

$$GO_2(G) = \sum_{uv \in E(G)} \big[\big(d_G(u) + d_G(v)\big)\big(d_G(u)d_G(v)\big)\big].$$

In [13], Kulli introduced the first and second hyper-Gourava indices of a molecular graph G which are defined as

$$HGO_1(G) = \sum_{uv \in E(G)} \big[d_G(u) + d_G(v) + d_G(u)d_G(v)\big]^2,$$

$$HGO_2(G) = \sum_{uv \in E(G)} \big[\big(d_G(u) + d_G(v)\big)\big(d_G(u)d_G(v)\big)\big]^2.$$

There are various research articles on Gourava and hyper-Gourava indices in literature, one can refer to [3, 4, 15]. Motivated by the definition of the Gourava indices, we introduce the first Basava index and second Basava index of graph as follows:

$$BA_1(G) = \sum_{uv \in E(G)} \big[S_G(u) + S_G(v) + S_G(u)S_G(v)\big],$$

$$BA_2(G) = \sum_{uv \in E(G)} \big[\big(S_G(u) + S_G(v)\big)\big(S_G(u)S_G(v)\big)\big].$$

Motivated by the definition of the hyper-Gourava indices, we introduce the first hyper-Basava index and second hyper-Basava index of graph as follows:

$$HBA_1(G) = \sum_{uv \in E(G)} \big[S_G(u) + S_G(v) + S_G(u)S_G(v)\big]^2,$$

$$HBA_2(G) = \sum_{uv \in E(G)} \big[\big(S_G(u) + S_G(v)\big)\big(S_G(u)S_G(v)\big)\big]^2.$$

The rest of the paper is organized as follows. In section 2, we obtain explicit formulae for the Basava and hyper-Basava indices of some graph families. In section 3, we study the chemical applicability of the Basava and hyper-Basava indices. In section 4, we derive the Basava and hyper-Basava indices of certain families of nanostar dendrimers.

2. Basava and hyper-Basava indices of some standard class of graphs

Theorem 2.1. *If G is an $r-$regular graph with n vertices, then*

(i) $BA_1(G) = \frac{nr^3}{2}[r^2 + 2]$,

(ii) $BA_2(G) = nr^7$,

(iii) $HBA_1(G) = \frac{nr^5}{2}[r^4 + 4r^2 + 4]$,

(iv) $HBA_2(G) = 2nr^{13}$.

Proof. If G is an $r-$regular graph with n vertices, then G has $\frac{nr}{2}$ edges. The degree sum of neighbours of each vertex of G is r^2. By the definition of the Basava and hyper-Basava indices, we get

(i) $BA_1(G) = \frac{nr}{2}[r^2 + r^2 + r^4] = \frac{nr^3}{2}[r^2 + 2]$.

(ii) $BA_2(G) = \frac{nr}{2}[(r^2 + r^2)r^4] = nr^7$.

(iii) $HBA_1(G) = \frac{nr}{2}[r^2 + r^2 + r^4]^2 = \frac{nr^5}{2}[r^4 + 4r^2 + 4]$.

(iv) $HBA_2(G) = \frac{nr}{2}[(r^2 + r^2)r^4]^2 = 2nr^{13}$.

Theorem 2.2. *Let P_n be a path with $n \geq 5$ vertices. Then*

(i) $BA_1(P_n) = 24n - 60$,

(ii) $BA_2(P_n) = 128n - 412$,

(iii) $HBA_1(P_n) = 576n - 1916$,

(iv) $HBA_2(P_n) = 16384n - 66008$.

Proof. Let $G = P_n$ be a path with $n \geq 5$ vertices. We obtain three partition of edge sets of P_n as follows:
$E_{2,3} = \{uv \in E(G)/S_G(u) = 2, S_G(v) = 3\}$, $|E_{2,3}| = 2$,
$E_{3,4} = \{uv \in E(G)/S_G(u) = 3, S_G(v) = 4\}$, $|E_{3,4}| = 2$,
$E_{4,4} = \{uv \in E(G)/S_G(u) = 4, S_G(v) = 4\}$, $|E_{4,4}| = n - 5$.
By using the definitions of Basava and hyper-Basava indices and edge partitions, we have

$$\begin{aligned} BA_1(P_n) &= \sum_{(u,v)\in E(G)} S_G(u) + S_G(v) + S_G(u)S_G(v) \\ &= |E_{2,3}|[(2+3) + (2\times 3)] + |E_{3,4}|[(3+4) + (3\times 4)] \\ &\quad +|E_{4,4}|[(4+4) + (4\times 4)] \\ &= 2[2+3+6] + 2[3+4+12] + (n-5)[4+4+16] \\ &= 24n - 60. \end{aligned}$$

$$\begin{aligned}
BA_2(P_n) &= \sum_{(u,v)\in E(G)} [(S_G(u)+S_G(v))(S_G(u)S_G(v))] \\
&= 2[(2+3)6]+2[(3+4)12]+(n-5)[(4+4)16] \\
&= 128n-412. \\
HBA_1(P_n) &= \sum_{(u,v)\in E(G)} (S_G(u)+S_G(v)+S_G(u)S_G(v))^2 \\
&= 2[2+3+6]^2+2[3+4+12]^2+(n-5)[4+4+16]^2 \\
&= 576n-1916. \\
HBA_2(P_n) &= \sum_{(u,v)\in E(G)} [(S_G(u)+S_G(v))(S_G(u)S_G(v))]^2 \\
&= 2[(2+3)6]^2+2[(3+4)12]^2+(n-5)[(4+4)16]^2 \\
&= 16384n-66008.
\end{aligned}$$

P_n	$BA_1(P_n)$	$BA_2(P_n)$	$HBA_1(P_n)$	$HBA_2(P_n)$
P_2	3	2	9	4
P_3	16	32	128	512
P_4	37	114	467	4716

Table 1: Basava and hyper-Basava indices of $P_n(n \leq 4)$.

Theorem 2.3. *Let $K_{m,n}$ be a complete bipartite graph with $1 \leq m \leq n$. Then*

(i) $BA_1(K_{m,n}) = m^2n^2(mn+2)$,

(ii) $BA_2(K_{m,n}) = 2m^4n^4$,

(iii) $HBA_1(K_{m,n}) = mn(2mn+m^2n^2)^2$,

(iv) $HBA_2(K_{m,n}) = 2m^7n^7$.

Proof. Let $G = K_{m,n}$ be a complete bipartite graph. We obtain one partition of edge set of $K_{m,n}$ as follows:
$E_1 = \{uv \in E(G)/S_G(u) = mn, S_G(v) = mn\}$, $|E_1| = mn$,
By using the definitions of Basava and hyper-Basava indices and edge partition, we obtain

$$\begin{aligned}
BA_1(K_{m,n}) &= \sum_{(u,v)\in E(K_{m,n})} S_G(u)+S_G(v)+S_G(u)S_G(v) \\
&= mn[mn+mn+m^2n^2] \\
&= m^2n^2(mn+2).
\end{aligned}$$

$$\begin{aligned}
BA_2(K_{m,n}) &= \sum_{(u,v)\in E(K_{m,n})} [(S_G(u)+S_G(v))(S_G(u)S_G(v))] \\
&= mn[(mn+mn)m^2n^2] \\
&= 2m^4n^4. \\
HBA_1(K_{m,n}) &= \sum_{(u,v)\in E(K_{m,n})} (S_G(u)+S_G(v)+S_G(u)S_G(v))^2 \\
&= mn[mn+mn+m^2n^2]^2 \\
&= mn(2mn+m^2n^2)^2. \\
HBA_2(K_{m,n}) &= \sum_{(u,v)\in E(K_{m,n})} [(S_G(u)+S_G(v))(S_G(u)S_G(v))]^2 \\
&= mn[(mn+mn)m^2n^2]^2 \\
&= 2m^7n^7.
\end{aligned}$$

Theorem 2.4. *Let $W_{1,n}$ be a wheel with $n \geq 3$ vertices. Then*

(i) $BA_1(W_{1,n}) = n[4n^2+36n+54]$,

(ii) $BA_2(W_{1,n}) = n[14n^3+126n^2+324n+432]$,

(iii) $HBA_1(W_{1,n}) = n[10n^4+160n^3+812n^2+1608n+2340]$,

(iv) $HBA_2(W_{1,n}) = 36n^3[2n^2+15n+18]^2 + 4n(n+6)^6$.

Proof. Let $G = W_{1,n}$ be a wheel with $n \geq 3$ vertices. We obtain three partition of edge sets of $W_{1,n}$ as follows:
$E_1 = \{uv \in E(G)/S_G(u) = 3n, S_G(v) = n+6\}$, $|E_1| = n$,
$E_2 = \{uv \in E(G)/S_G(u) = n+6, S_G(v) = n+6\}$, $|E_2| = n$,
By using the definitions of Basava and hyper-Basava indices and edge partitions, we get

$$\begin{aligned}
BA_1(W_{1,n}) &= \sum_{(u,v)\in E(W_{1,n})} S_G(u)+S_G(v)+S_G(u)S_G(v) \\
&= n[3n+n+6+3n(n+6)] + n[n+6+n+6+(n+6)^2] \\
&= n[4n^2+36n+54].
\end{aligned}$$

$$\begin{aligned}
BA_2(W_{1,n}) &= \sum_{(u,v)\in E(W_{1,n})} [(S_G(u)+S_G(v))(S_G(u)S_G(v))] \\
&= n[(3n+n+6)3n(n+6)] + n[(n+6+n+6)(n+6)^2] \\
&= n[14n^3+126n^2+324n+432].
\end{aligned}$$

$$\begin{aligned} HBA_1(W_{1,n}) &= \sum_{(u,v)\in E(W_{1,n})} (S_G(u)+S_G(v)+S_G(u)S_G(v))^2 \\ &= n[3n+n+6+3n(n+6)]^2+n[n+6+n+6+(n+6)^2]^2 \\ &= n[10n^4+160n^3+812n^2+1608n+2340]. \end{aligned}$$

$$\begin{aligned} HBA_2(W_{1,n}) &= \sum_{(u,v)\in E(W_{1,n})} [(S_G(u)+S_G(v))(S_G(u)S_G(v))]^2 \\ &= n[(3n+n+6)3n(n+6)]^2+n[(n+6+n+6)(n+6)^2]^2 \\ &= 36n^3[2n^2+15n+18]^2+4n(n+6)^6. \end{aligned}$$

The following theorem gives the relationship between the Basava and hyper-Basava indices are expressed interims of other topological indices which are already in the literature.

Theorem 2.5. *Let G be a graph with n vertices and m edges. Then*

1. $BA_1(G) = M_1G_5(G) + M_2G_5(G)$,
2. $HBA_1(G) = HM_1G_5(G) + HM_2G_5(G) + BA_2(G)$.

Proof. 1. By using the definition of first Basava index, we have

$$\begin{aligned} BA_1(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u)+S_G(v)\big)+\big(S_G(u)S_G(v)\big)\big] \\ &= \sum_{(u,v)\in E(G)} \big(S_G(u)+S_G(v)\big)+\sum_{(u,v)\in E(G)} \big(S_G(u)S_G(v)\big) \\ &= M_1G_5(G)+M_2G_5(G). \end{aligned}$$

2. By using the definition of first hyper-Basava index, we have

$$\begin{aligned} HBA_1(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u)+S_G(v)\big)+\big(S_G(u)S_G(v)\big)\big]^2 \\ &= \sum_{(u,v)\in E(G)} \big(S_G(u)+S_G(v)\big)^2+\sum_{(u,v)\in E(G)} \big(S_G(u)S_G(v)\big)^2 \\ &\quad + \sum_{(u,v)\in E(G)} 2\big(S_G(u)+S_G(v)\big)\big(S_G(u)S_G(v)\big) \\ &= HM_1G_5(G)+HM_2G_5(G)+2BA_2(G). \end{aligned}$$

3. Chemical applicability of Basava and hyper-Basava indices of graphs

In this section, we present a linear regression model of these physical properties with the Basava and hyper-Basava indices. Basava and hyper-Basava indices are neighbourhood degree based indices. These indices have good correlation with physical properties of chemical compounds like entropy(S), acentric factor(AcentFac) and standard enthalpy of vaporization(DHVAP) of octane isomers. Basava and hyper-Basava indices are tested using a data set of octane isomers found at http://www.moleculardescriptors.eu/dataset.htm. The columns 5, 6, 7 and 8 of Table 2 are computed by using the definition of first Basava index, second Basava index, first hyper-Basava indices and second hyper-Basava index, respectively.

Alkane	S	AcentFac	DHVAP	BA_1	BA_2	HBA_1	HBA_2
n-octane	111.67	0.397898	9.915	132	612	2692	65064
2-methyl-heptane	109.84	0.377916	9.484	150	770	3462	103252
3-methyl-heptane	111.26	0.371002	9.521	160	892	4114	151960
4-methyl-heptane	109.32	0.371504	9.483	161	920	4279	170000
3-ethyl-hexane	109.43	0.362472	9.476	161	960	4533	211248
2, 2-dimethyl-hexane	103.42	0.339426	8.915	192	1224	5842	271656
2, 3-dimethyl-hexane	108.02	0.348247	9.272	189	1212	5799	288144
2, 4-dimethyl-hexane	106.98	0.344223	9.029	179	1086	5125	229716
2, 5-dimethyl-hexane	105.72	0.35683	9.051	169	946	4351	155524
3, 3-dimethyl-hexane	104.74	0.322596	8.973	212	1504	7436	442768
3, 4-dimethyl-hexane	106.59	0.340345	9.316	182	1128	5328	135252
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	199	1352	6701	399536
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	231	1778	9015	638764
2, 2, 3-trimethyl-pentane	101.31	0.300816	8.826	241	1832	9171	612184
2, 2, 4-trimethyl-pentane	104.09	0.30537	8.402	211	1436	6975	382576
2, 3, 3-trimethyl-pentane	102.06	0.293177	8.897	251	1976	10023	721632
2, 3, 4-trimethyl-pentane	102.39	0.317422	9.014	217	1530	7495	454500
2, 2, 3, 3-tetramethyl-butane	93.06	0.255294	8.41	346	3122	16574	1560404

Table 2: Experimental values of entropy, acentric factor, DHVAP and the corresponding values of first Basava index, second Basava index, first hyper-Basava index and second hyper-Basava index of octane isomers.

The linear regression models for entropy, acentic factor and DHVAP using the data of Tables 2 are obtained using the least squares fitting procedure as implemented in R software [17].

The fitted models for BA_1 are:

$$S = 123.01(\pm 1.34) - 0.1(\pm 0.006)BA_1 \tag{2.1}$$

$$AcentFac = 0.5(\pm 0.01) - 0.0007(\pm 0.00005)BA_1 \tag{2.2}$$

$$DHVAP = 10.4(\pm 0.24) - 0.006(\pm 0.0012)BA_1 \tag{2.3}$$

The fitted models for BA_2 are:

$$S = 115.4(\pm 0.9) - 0.0074(\pm 0.0006)BA_2 \tag{2.4}$$
$$AcentFac = 4.138e-01(\pm 0.007) - 0.00006(\pm 0.000005)BA_2 \tag{2.5}$$
$$DHVAP = 9.81(\pm 0.15) - 0.00051(\pm 0.00011)BA_2 \tag{2.6}$$

The fitted models for HBA_1 are:

$$S = 114.2(\pm 0.84) - 0.0013(\pm 0.00011)HBA_1 \tag{2.7}$$
$$AcentFac = 0.4(\pm 0.0068) - 0.00001(\pm 0.0000009)HBA_1 \tag{2.8}$$
$$DHVAP = 9.723(\pm 0.14) - 0.00009(\pm 0.00002)HBA_1 \tag{2.9}$$

The fitted models for HBA_2 are:

$$S = 110(\pm 0.68) - 0.000012(\pm 0.0000013)HBA_2 \tag{2.10}$$
$$AcentFac = 0.3(\pm 0.006) - 0.00000009(\pm 0.000000012)HBA_2 \tag{2.11}$$
$$DHVAP = 9.423(\pm 0.1) - 0.0000008(\pm 0.0000002)HBA_2 \tag{2.12}$$

Note. The values in brackets of Eqns. (2.1) to (2.12) are the corresponding standard errors of the regression coefficients. The index is better as $|r|$ approaches 1.

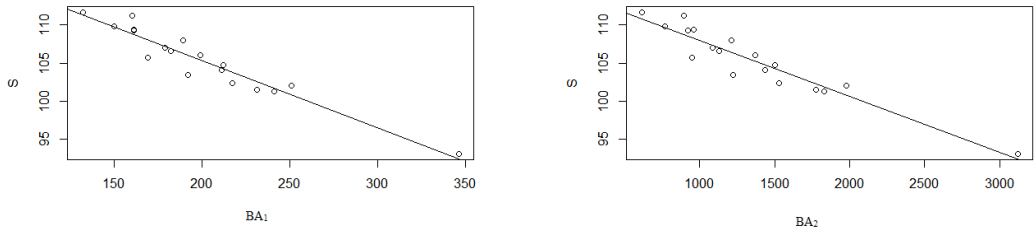

Figure 1: Scatter diagram of S on BA_1(left) and BA_2(right), superimposed by the fitted regression line.

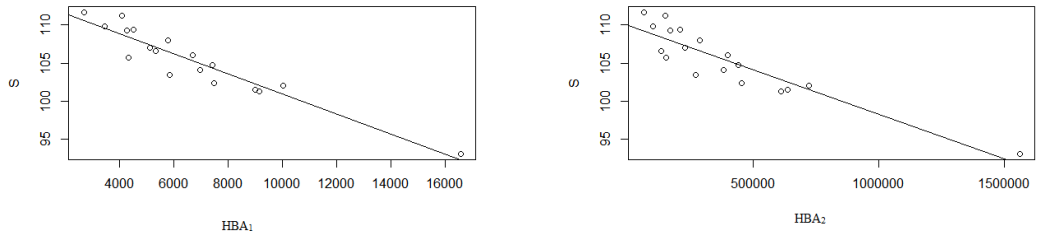

Figure 2: Scatter diagram of S on HBA_1(left) and HBA_2(right), superimposed by the fitted regression line.

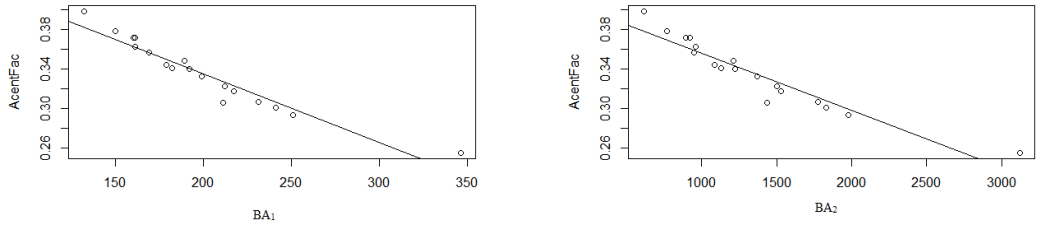

Figure 3: Scatter diagram of Acent Fac on BA_1(left) and BA_2(right), superimposed by the fitted regression line.

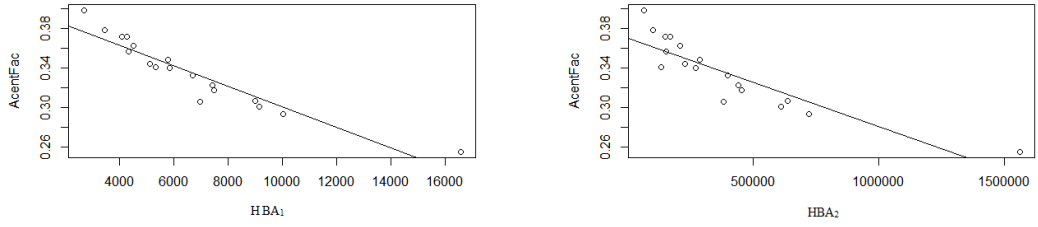

Figure 4: Scatter diagram of Acent Fac on HBA_1(left) and HBA_2(right), superimposed by the fitted regression line.

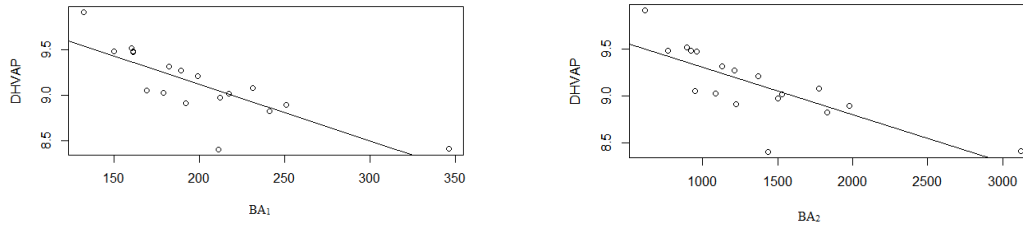

Figure 5: Scatter diagram of DHVAP on BA_1(left) and BA_2(right), superimposed by the fitted regression line.

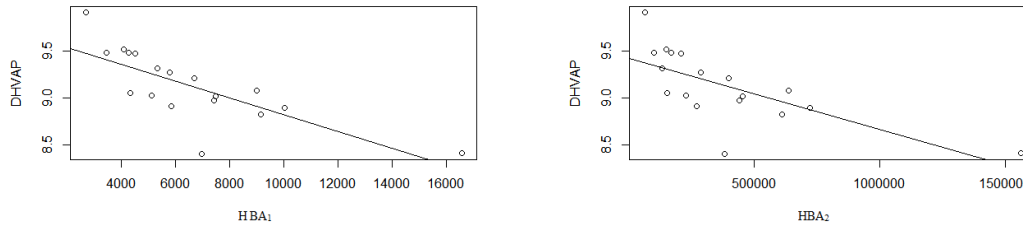

Figure 6: Scatter diagram of DHVAP on HBA_1(left) and HBA_2(right), superimposed by the fitted regression line.

Physical property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Entropy	**0.9585874**	1.326
Acentric Factor	**0.9590748**	0.01035
DHVAP	0.8008941	0.2366

Table 3: Correlation coefficient and residual standard error of regression models for BA_1.

Physical property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Entropy	**0.9491009**	1.467
Acentric Factor	**0.9485644**	0.01157
DHVAP	0.770291	0.252

Table 4: Correlation coefficient and residual standard error of regression models for BA_2.

Physical property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Entropy	**0.945135**	1.521
Acentric Factor	**0.9410579**	0.01236
DHVAP	0.75881758	0.2573

Table 5: Correlation coefficient and residual standard error of regression models for HBA_1.

Physical property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Entropy	**0.9128851**	1.901
Acentric Factor	0.8862783	0.01692
DHVAP	0.6999044	0.2822

Table 6: Correlation coefficient and residual standard error of regression models for HBA_2.

From Table 3, Figs. 1, 3 and 5 we can observe that BA_1 correlates highly with entropy (correlation coefficient $|r| = 0.9585874$) and Acentric Factor (correlation coefficient $|r| = 0.9590748$). Also, BA_1 has good correlation ($|r|>0.8$) with DHVAP.
From Table 4, Figs. 1, 3 and 5 we can observe that BA_2 correlates highly with entropy (correlation coefficient $|r| = 0.9491009$) and Acentric Factor (correlation coefficient $|r| = 0.9485644$). Also, ($|r|>0.75$) with DHVAP.
From Table 5, Figs. 2, 4 and 6 we can observe that HBA_1 correlates highly with entropy (correlation coefficient $|r| = 0.945135$) and Acentric Factor (correlation coefficient $|r| = 0.9410579$). Also, ($|r|>0.75$) with DHVAP.
From Table 6, Figs. 2, 4 and 6 HBA_2 has good correlation ($|r|>0.9$) with entropy, ($|r|>0.85$) with Acentric Factor and ($|r|>0.65$) with DHVAP.
Figure 7 gives comparison of r values for different physico-chemical properties like Entropy, Acentric Factor and DHVAP.

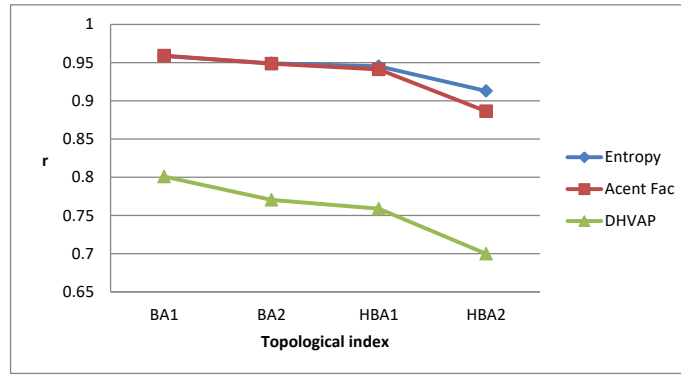

Figure 7: Plot of r values for Entropy, Acentric Factor and DHVAP

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4. Basava and hyper-Basava indices of certain families of nanostar dendrimers

In this section, we compute Basava and hyper-Basava indices of some families of nanostar dendrimers. The PAMAM dendrimer of generation G_n with n growth stages, denoted by $PD_1[n]$ where $n \geq 0$. The number of vertices and edges in $PD_1[n]$ are $12 \times 2^{n+2} - 23$ and $12 \times 2^{n+2} - 24$(see [1]). The graph $PD_1[3]$ is depicted in figure 8.

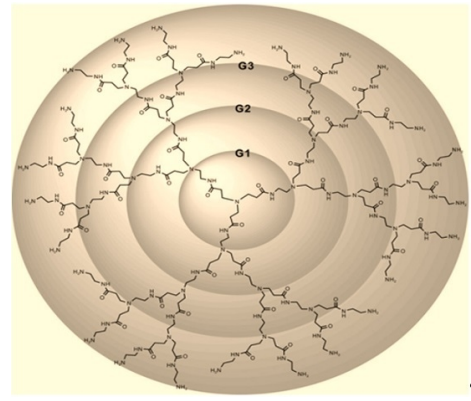

Figure 8: PAMAM dendrimer of generations G_n with growth stages, $PD_1[3]$.

(S_u, S_v) **where** $uv \in E(G)$	**Number of edges**
$(2, 3)$	3×2^n
$(3, 4)$	3×2^n
$(3, 5)$	$6 \times 2^n - 3$
$(4, 5)$	$9 \times 2^n - 6$
$(5, 5)$	$18 \times 2^n - 9$
$(5, 6)$	$9 \times 2^n - 6$

Table 7: Edge partition of PAMAM dendrimer, $PD_1[n]$ based on degree sum neighbours of end vertices of each edge.

Theorem 4.1. *Let G be a PAMAM dendrimer $PD_1[n]$. Then*

1. $BA_1(G) = 1488 \times 2^n - 804$,

2. $BA_2(G) = 7551 \times 2^n - 3936$,

3. $HBA_1(G) = 49368 \times 2^n - 27744$,

4. $HBA_2(G) = 529497 \times 2^n - 810186$.

Proof. Let G be a PAMAM dendrimer $PD_1[n]$.
By using the definitions of Basava and information in Table 7, we have

$$\begin{aligned} BA_1(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u) + S_G(v)\big) + \big(S_G(u)S_G(v)\big)\big] \\ &= (3 \times 2^n)(2+3+6) + (3 \times 2^n)(3+4+12) \\ &\quad +(6 \times 2^n - 3)(3+5+15) + (9 \times 2^n - 6)(4+5+20) \\ &\quad +(18 \times 2^n - 9)(5+5+25) + (9 \times 2^n - 6)(5+6+30) \\ &= 1488 \times 2^n - 804. \end{aligned}$$

2. By using the definition of second Basava index and information in Table 7, we have

$$\begin{aligned} BA_2(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u) + S_G(v)\big)\big(S_G(u)S_G(v)\big)\big] \\ &= (3 \times 2^n)[(2+3)6] + (3 \times 2^n)[(3+4)12] \\ &\quad +(6 \times 2^n - 3)[(3+5)15] + (9 \times 2^n - 6)[(4+5)20] \\ &\quad +(18 \times 2^n - 9)[(5+5)25] + (9 \times 2^n - 6)[(5+6)30] \\ &= 10152 \times 2^n - 5670. \end{aligned}$$

3. By using the definition of first hyper-Basava index and information in Table 7, we have

$$\begin{aligned} HBA_1(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u) + S_G(v)\big) + \big(S_G(u)S_G(v)\big)\big]^2 \\ &= (3 \times 2^n)(2+3+6)^2 + (3 \times 2^n)(3+4+12)^2 \\ &\quad +(6 \times 2^n - 3)(3+5+15)^2 + (9 \times 2^n - 6)(4+5+20)^2 \\ &\quad +(18 \times 2^n - 9)(5+5+25)^2 + (9 \times 2^n - 6)(5+6+30)^2 \\ &= 49368 \times 2^n - 27744. \end{aligned}$$

4. By using the definition of second hyper-Basava index and information in Table

7, we have

$$\begin{aligned} HBA_2(G) &= \sum_{(u,v)\in E(G)} \big[\big(S_G(u)+S_G(v)\big)\big(S_G(u)S_G(v)\big)\big]^2 \\ &= (3\times 2^n)[(2+3)6]^2+(3\times 2^n)[(3+4)12]^2 \\ &\quad +(6\times 2^n-3)[(3+5)15]^2+(9\times 2^n-6)[(4+5)20]^2 \\ &\quad +(18\times 2^n-9)[(5+5)25]^2+(9\times 2^n-6)[(5+6)30]^2 \\ &= 2506968\times 2^n-1453500. \end{aligned}$$

We shall now determine the Basava and hyper-Basava indices of tetrathiafulvalene dendrimer of generation G_n with n growth stages, denoted by $TD_2[n]$ where $n \geq 0$. The graph of $TD_2[n]$bhas $31\times 2^{n+2}-74$ vertices and $35\times 2^{n+2}-85$ edges as shown in Figure 9.

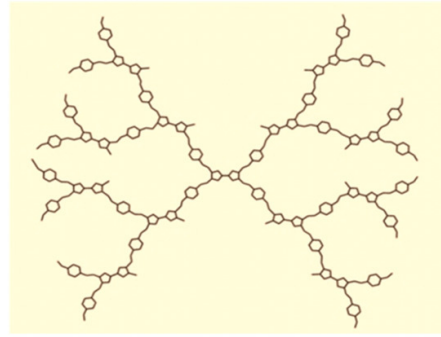

Figure 9: Tetrathiafulvalene dendrimer with 2−growth stages, $TD_2[2]$

(S_u, S_v) **where** $uv \in E(G)$	**Number of edges**
$(2,4)$	2^{n+2}
$(3,6)$	$2^{n+2}-4$
$(4,6)$	2^{n+2}
$(5,5)$	$7\times 2^{n+2}-16$
$(5,6)$	$11\times 2^{n+2}-24$
$(5,7)$	$3\times 2^{n+2}-8$
$(6,6)$	$2^{n+2}-4$
$(6,7)$	$8\times 2^{n+2}-24$
$(7,7)$	$2\times 2^{n+2}-5$

Table 8: Edge partition of tetrathiafulvalene dendrimer, $TD_2[n]$ based on degree sum neighbours of end vertices of each edge.

Theorem 4.2. *Let G be a tetrathiafulvalene dendrimer $TD_2[n]$. Then*

1. $BA_1(G) = 1526 \times 2^{n+2} - 3855$,
2. $BA_2(G) = 13262 \times 2^{n+2} - 34190$,
3. $HBA_1(G) = 70216 \times 2^{n+2} - 182193$,
4. $HBA_2(G) = 5763492 \times 2^{n+2} - 15384036$.

Proof. Let G be a tetrathiafulvalene dendrimer $TD_2[n]$.
By using the definitions of Basava and hyper-Basava indices and information in Table 8, we get the required result. The proof is similar to Theorem 4.1.

Now, we study Basava and hyper-Basava indices of POPAM dendrimers, denoted by $POD_2[n]$ where $n \geq 0$. The number of vertices and edges in $POD_2[n]$ are $2^{n+5} - 10$ and $2^{n+5} - 11$, respectively (see 2). The POPAM dendrimer $POD_2[n]$ with 2 growth stages is shown in Figure 10.

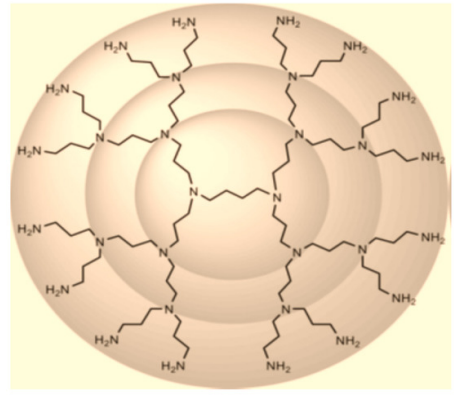

Figure 10: POPAM dendrimer of generations G_n with two growth stages, $POD_2[2]$.

(S_u, S_v) **where** $uv \in E(G)$	**Number of edges**
$(2, 3)$	2^{n+2}
$(3, 4)$	2^{n+2}
$(4, 4)$	1
$(4, 5)$	$3 \times 2^{n+2} - 6$
$(5, 6)$	$3 \times 2^{n+2} - 6$

Table 9: Edge partition of POPAM dendrimer, $POD_2[n]$ based on degree sum neighbours of end vertices of each edge.

Theorem 4.3. *Let G be a POPAM dendrimer $POD_2[n]$. Then*

1. $BA_1(G) = 240 \times 2^{n+2} - 396$,
2. $BA_2(G) = 1644 \times 2^{n+2} - 2932$,
3. $HBA_1(G) = 8048 \times 2^{n+2} - 14556$,
4. $HBA_2(G) = 431856 \times 2^{n+2} - 831416$.

Proof. Let G be a POPAM dendrimer $POD_2[n]$.
By using the definitions of Basava and hyper-Basava indices and information in Table 9, we get the required result. The proof is similar to Theorem 4.1.

5. Comparative Analysis

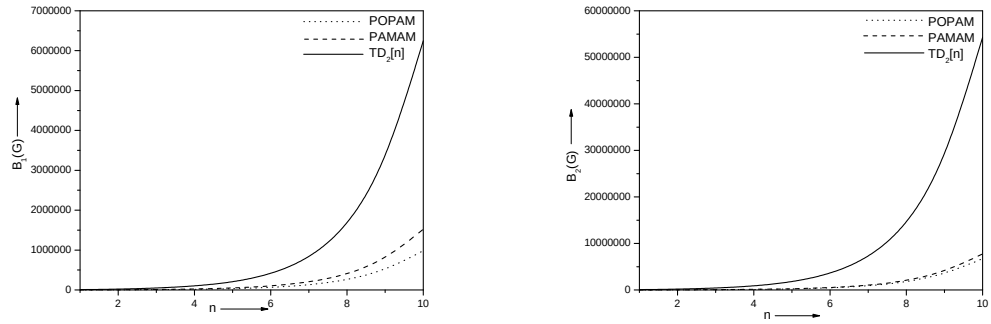

Figure 11: Plot of $BA_1(G)$(left) and $BA_2(G)$(right) for dendrimers.

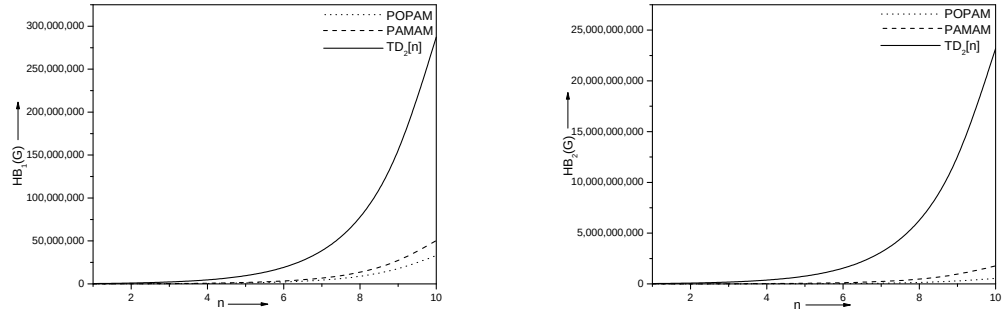

Figure 12: Plot of $HBA_1(G)$(left) and $HBA_2(G)$(right) for dendrimers.

Figures 11 and 12 shows that $BA_1(PAMAM)$, $BA_2(PAMAM)$, $HBA_1(PAMAM)$, $HBA_2(PAMAM)$, $BA_1(TD_2[n])$, $BA_2(TD_2[n])$, $HBA_1(TD_2[n])$, $HBA_2(TD_2[n])$, $BA_1(POPAM)$, $BA_2(POPAM)$, $HBA_1(POPAM)$, $HBA_2(POPAM)$ are exponentially increasing. Figure 11 shows that the saturation points are close for $BA_2(PAMAM)$ and $BA_2(POPAM)$.

6. Conclusion

In this paper, we have introduced a novel topological indices namely the Basava indices and hyper-Basava indices of a molecular graph. We computed the Basava and hyper-Basava indices of some standard class of graphs. The Basava and hyper-Basava indices are tested with physico-chemical properties of octane isomers such as entropy, acentric factor and DHVAP using linear regression models. The first Basava index highly correlates with acentric factor (coefficient of correlation **0.9590748**) which is better than the neighborhood version of forgotten topological index(coefficient of correlation **0.93831**) [16] and the second Basava index highly correlates with entropy (coefficient of correlation **0.9491009**). We derived the analytical closed formulae for certain families of nanostar dendrimers. The obtained results can be used in data mining, particularly in researching the uniqueness of hyper-branched molecular graphs.

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