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Analysis of closed neighbourhood indices of some networks - II

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Abstract

Topological indices are extensively used for establishing relationship between the chemical structure and their physico-chemical properties. Motivated by chemical applications of topological indices in the QSPR/QSAR analysis, we introduce a new topological indices that we call, *second BM Index* and *fourth BM Index*, is denoted by $BM_2(G)$ and $BM_4(G)$. Also we introduce *second and fourth BM polynomials* and is denoted by $BM_2(G,x)$ and $BM_4(G,x)$. In this paper, $BM_2(G)$ and $BM_4(G)$ is tested with physico-chemical properties of octane isomers such as entropy, acentric factor, enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) using the linear models. The $BM_2(G)$ and $BM_4(G)$ shows excellent correlation with these chemical properties. Specially, $BM_2(G)$ and $BM_4(G)$ highly correlates with acentric factor (coefficient of correlation 0.9906546 and 0.9783643). Furthermore, we obtain $BM_2(G)$, $BM_4(G)$ indices and $BM_2(G,x)$, $BM_4(G,x)$ polynomials of dominating oxide network, regular triangulate oxide network, H-Naphtalenic nanotubes and nanocones of molecular graphs.

Keywords: *BM* indices, nanostructures, closed neighbourhood indices.
2010 MSC: 05C05, 05C12, 05C35.

1. Introduction and Preliminaries

Let $G = (V, E)$ be a finite, undirected graph without loops and multiple edges with V as vertex set and E as edge set. Let $|V| = n$ and $|E| = m$. The vertices and the edges of G are used to represent the atoms and the bonds of chemical structures. For a graph G, the neighbourhood of a vertex $u \in V(G)$ is defined as the $N_G(u)$ consisting of all points v which are adjacent with u. The closed neighbourhood is $N_G[u] = N_G(u) \cup \{u\}$. The degree of a vertex $u \in V(G)$, denoted by $d_G(u)$ and defined as $|N_G(u)|$. Let $S_G(u) = \sum_{u \in N_G(u)} d_G(v)$ be the degree sum of neighbourhood vertices. The closed neighbourhood [6]

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degree sum of vertices denoted by $S_G[u]$ and defined as $S_G[u] = \sum_{u \in N_G(u)} d_G(v)$. For unexplained graph terminology and notation refer [10, 12].

Recently, we have [7], proposed closed neighbouhood degree based topological indices, which are first and third BM indices and polynomials of a molecular graph G, defined as follows.

The first and third BM indices of a molecular graph G [7] is defined as

$$BM_1(G) = \sum_{uv \in E(G)} \frac{S_G[u] + S_G[v]}{2},$$

$$BM_3(G) = \sum_{uv \in E(G)} \left(\frac{S_G[u] + S_G[v]}{2} \right)^2.$$

The first and third BM polynomials of a molecular graph G [7] is defined as

$$BM_1(G, x) = \sum_{uv \in E(G)} x^{\frac{S_G[u]+S_G[v]}{2}}$$

,

$$BM_3(G, x) = \sum_{uv \in E(G)} x^{\left(\frac{S_G[u]+S_G[v]}{2}\right)^2}.$$

Motivated by the recent results on chemical structures and its applications, we now introduce the second and fourth BM indices of the molecular graph G as follows.

The second BM index of a molecular graph G is defined as

$$BM_2(G) = \sum_{uv \in E(G)} \frac{S_G[u]S_G[v]}{2}.$$

The fourth BM index of a molecular graph G is defined as

$$BM_4(G) = \sum_{uv \in E(G)} \left(\frac{S_G[u]S_G[v]}{2} \right)^2.$$

Next, we introduce the second and fourth BM polynomials of a molecular graph as follows.

The second BM polynomial of a molecular graph G is defined as

$$BM_2(G, x) = \sum_{uv \in E(G)} x^{\frac{S_G[u]S_G[v]}{2}}.$$

The fourth BM polynomial of a molecular graph G is defined as

$$BM_4(G, x) = \sum_{uv \in E(G)} x^{\left(\frac{S_G[u]S_G[v]}{2}\right)^2}.$$

In the literature, many researchers studied the topological indices of molecular graphs which are in [1, 2, 5, 7, 8, 9, 11, 14, 15, 16, 18]. Kulli [13] studied neighborhood Sombor index of nanostructures. First time Basavanagoud et. al [6] introduced Chinmayi indices (closed neighbourhood degree indices) of graphs. Motivated by this [6], we obtain $BM_2(G)$, $BM_4(G)$ indices and $BM_2(G, x)$, $BM_4(G, x)$ polynomials of dominating oxide network, regular triangulate oxide network, H-Naphtalenic nanotubes and nanocones of molecular graphs.

The molecular weight, volume, pressure, density, and refraction of organic compounds, as well as their boiling, freezing, and vaporisation points, isomer and edge shift, infrared group frequency, quadruple splitting, and polarizability, can all be determined using topological indices.

2. On the chemical applicability of $BM_2(G)$ and $BM_4(G)$ indices on octane isomers

In this section, we discuss the linear regression analysis of $BM_2(G)$ and $BM_4(G)$ with entropy(S), acentric factor(AcentFac), enthalpy of vaporization(HVAP) and DHVAP of octane isomers. The $BM_2(G)$ and $BM_4(G)$ was tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. Interestingly, we have noticed that $BM_2(G)$ and $BM_4(G)$ indices are highly correlated with acentric factor (AcentFac) ($|r|$=**0.9906546** and $|r|$=**0.9783643**). The dataset of octane isomers (columns 1-5 of Table 1) are taken from above web link whereas the 6^{th} and 7^{th} columns of Table 1 is calculated by definition of $BM_2(G)$ and $BM_4(G)$ indices.

Table 1: Some physical properties and $BM_2(G)$, $BM_4(G)$ indices of octane isomers.

Alkane	**S**	**AcentFac**	**DHVAP**	**HVAP**	$BM_2(G)$	$BM_4(G)$
n-octane	111.67	0.397898	9.915	73.19	99	1534.5
2-methyl-heptane	109.84	0.377916	9.484	70.3	114	2038.5
3-methyl-heptane	111.26	0.371002	9.521	71.3	120.5	2419.25
4-methyl-heptane	109.32	0.371504	9.483	70.91	122	2549
3-ethyl-hexane	109.43	0.362472	9.476	71.7	128.5	2974.75
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	150	3672
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	149	2938.5
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	137	3113
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	129.5	2584.75
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	163	4641.5
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	148.5	3908.25
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	150	4074
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	174.5	5533.75
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	184	5756
2,2,4-trimethyl-pentane	104.09	0.30537	8.402	64.87	167.5	4543.25
2,3,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	189.5	6203.25
2,3,4-trimethyl-pentane	102.39	0.317422	9.014	68.37	164	4624
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	225.5	8198

The linear regression models for the entropy, acentric factor, DHVAP and HVAP using the data of Table 1 are obtained using the least squares fitting procedure as implemented in R software [17]. The $BM_2(G)$ fitted models are:

$$S = 126.29475(\pm 1.78752) - 0.13839(\pm 0.01162)BM_2(G) \quad (2.1)$$

$$AcentFac = 0.5070(\pm 0.006010) - 0.001135(\pm 0.00003906)BM_2(G) \quad (2.2)$$

$$DHVAP = 10.707271(\pm 0.254125) - 0.010477(\pm 0.001652)BM_2(G) \quad (2.3)$$

$$HVAP = 76.72436(\pm 1.62116) - 0.05011(\pm 0.01054)BM_2(G) \quad (2.4)$$

Note: The values in the brackets of Eqs. (2.1) to (2.4) are the corresponding standard errors of the regression coefficients.

From Table 2, we can observe that $BM_2(G)$ highly correlates with acentric factor which is better than first Zagreb index ($|r|$=0.973087869 and residual standard error is 0.008424), second order first Zagreb index ($|r|$=0.99020 and residual standard error is 0.005101)[3] and $(\beta, \alpha)-$connectivity index ($|r|$=0.95802 and residual standard error is 0.01047) [4]. Closer the $|r|$ to 1, better is the index.

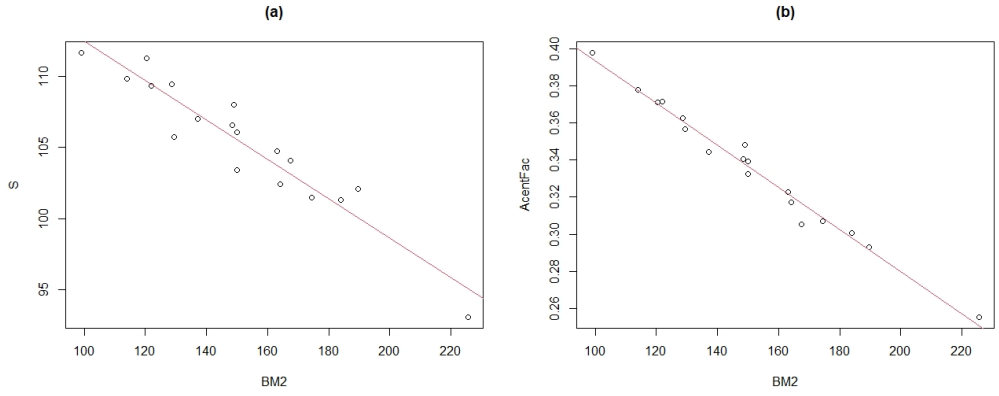

Figure 1: Scatter diagram of (a) S on $BM_2(G)$, (b) $AcentFac$ on $BM_2(G)$, superimposed by the fitted regression line.

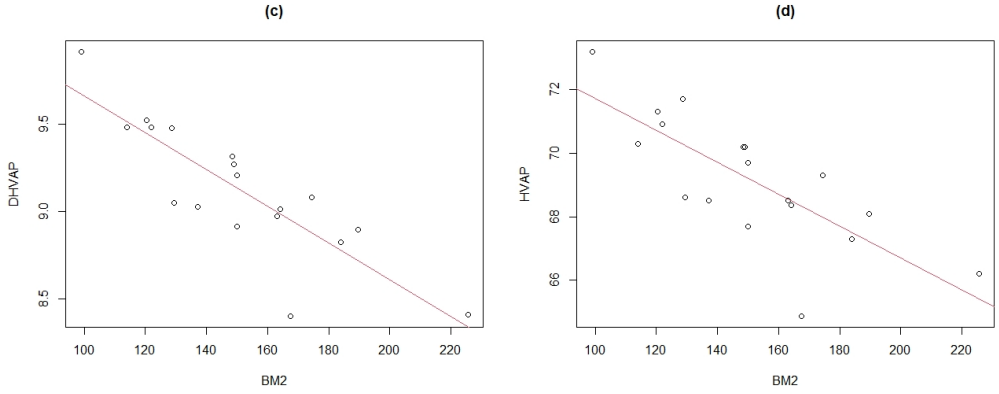

Figure 2: Scatter diagram of (c) $DHVAP$ on $BM_2(G)$ (d) $HVAP$ on $BM_2(G)$, superimposed by the fitted regression line.

Table 2: Correlation coefficient and residual standard error of regression models

Physical Property	**Absolute value of the correlation coefficient ($\|r\|$)**	**Residual standard error**
Enthalpy	0.9479773	1.482
Acentric Factor	**0.9906546**	**0.004984**
DHVAP	0.8458742	0.2107
HVAP	0.7652918	1.344

The BM_4 fitted models are:

$$S = 115.4(\pm 0.9404) - 0.002524(\pm 0.0002193)BM_4(G) \quad (2.5)$$

$$AcentFac = 0.4170(\pm 0.004651) - 0.00002051(\pm 0.000001084)BM_4(G) \quad (2.6)$$

$$DHVAP = 9.837(\pm 0.1485) - 0.0001794(\pm 0.00003464)BM_4(G) \quad (2.7)$$

$$HVAP = 72.5099144(\pm 0.9113208) - 0.0008448(\pm 0.0002125)BM_4(G) \quad (2.8)$$

Note: The values in the brackets of Eqs. (2.5) to (2.8) are the corresponding standard errors of the regression coefficients.

From Table 3, we can observe that $BM_4(G)$ also highly correlates with acentric factor.

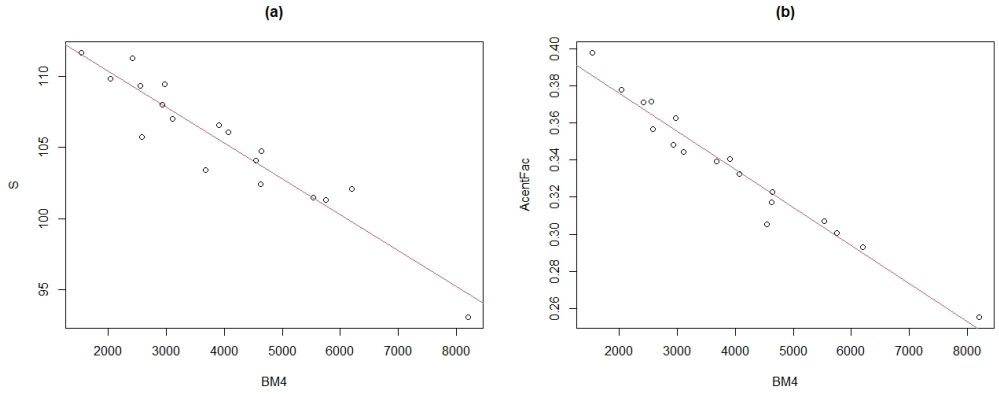

Figure 3: Scatter diagram of (a) S on $BM_4(G)$, (b) $AcentFac$ on $BM_4(G)$, superimposed by the fitted regression line.

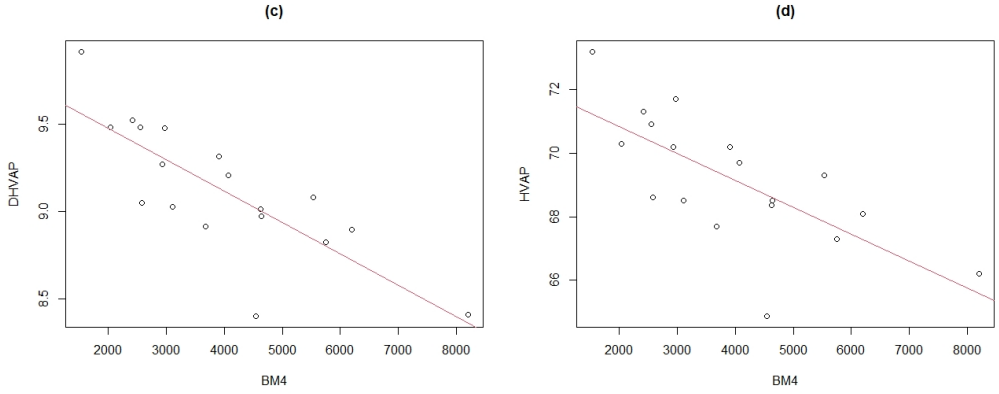

Figure 4: Scatter diagram of (c) $DHVAP$ on $BM_4(G)$ (d) $HVAP$ on $BM_4(G)$, superimposed by the fitted regression line.

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

Physical Property	**Absolute value of the correlation coefficient ($\|r\|$)**	**Residual standard error**
Enthalpy	0.9445771	1.529
Acentric Factor	**0.9783643**	**0.00756**
DHVAP	0.7915089	0.2415
HVAP	0.7049417	1.481

3. Results for Dominating Oxide Network $DOX(n)$

In this section, we consider the graph of a dominating oxide network $DOX(n)$, see Figure 5.

Let G be the graph of $DOX(n)$. The graph dominating oxide network $DOX(n)$ has $54n^2 - 54n + 18$ edges. Also there are two types of edges in G based on the degrees of end vertices of each edge as follows:

$$E_1 = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 4\}, \qquad |E_1| = 24n - 12,$$
$$E_2 = \{uv \in E(G) | d_G(u) = d_G(v) = 4\}, \qquad |E_2| = 54n^2 - 78n + 30.$$

The partition of the edges with respect to their sum degree of end vertices of dominating oxide network is given in Table 4.

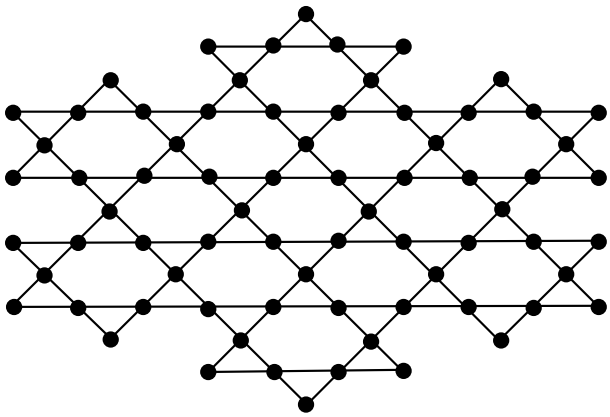

Figure 5: Dominating oxide network $DOX(2)$.

Table 4: Edge partition of dominating oxide network $DOX(n)$.

$(S_G[u], S_G[v])$	(10, 16)	(10, 18)	(16, 16)	(16, 18)	(18, 20)	(20, 20)
Number of edges	$12n$	$12n-12$	6	$12n-12$	$24n-24$	$54n^2-114n+60$

In the following theorems, we obtain explicit formulae for computing $BM_2(G)$, $BM_4(G)$, $BM_2(G,x)$ and $BM_4(G,x)$ of the dominating oxide network $DOX(n)$.

Theorem 3.1. *Let $DOX(n)$ be the family of dominating oxide network. Then*

1. $BM_2(DOX(n)) = 10800n^2 - 14712n + 5640$.
2. $BM_4(DOX(n)) = 2160000n^2 - 335968n + 1374672$.

Proof. We give the proof for one of the topological graph indices under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 4. Then

$$\begin{aligned} BM_2(G) &= \sum_{uv\in E(G)} \frac{S_G[u]S_G[v]}{2} \\ &= m_{10,16}\left(\frac{10\times 16}{2}\right) + m_{10,18}\left(\frac{10\times 18}{2}\right) + m_{16,16}\left(\frac{16\times 16}{2}\right) \\ &+ m_{16,18}\left(\frac{16\times 18}{2}\right) + m_{18,20}\left(\frac{18\times 20}{2}\right) + m_{20,20}\left(\frac{20\times 20}{2}\right) \\ &= 10800n^2 - 14712n + 5640. \end{aligned}$$

□

Theorem 3.2. *Let $DOX(n)$ be the family of dominating oxide network. Then*

1. $BM_2(DOX(n),x) = 12nx^{80} + (12n-12)x^{90} + 6x^{128} + (12n-12)x^{144} + (24n-24)x^{180} + (54n^2-114n+60)x^{200}$.
2. $BM_4(DOX(n),x) = 12nx^{6400} + (12n-12)x^{8100} + 6x^{16384} + (12n-12)x^{20736} + (24n-24)x^{32400} + (54n^2-114n+60)x^{40000}$.

Proof. We give the proof for one of the topological graph polynomial under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 4. Then

$$\begin{aligned} BM_2(G,x) &= \sum_{uv\in E(G)} x^{\frac{S_G[u]S_G[v]}{2}} \\ &= m_{10,16}x^{\left(\frac{10\times 16}{2}\right)} + m_{10,18}x^{\left(\frac{10\times 18}{2}\right)} + m_{16,16}x^{\left(\frac{16\times 16}{2}\right)} \\ &+ m_{16,18}x^{\left(\frac{16\times 18}{2}\right)} + m_{18,20}x^{\left(\frac{18\times 20}{2}\right)} + m_{20,20}x^{\left(\frac{20\times 20}{2}\right)} \\ &= 12nx^{80} + (12n-12)x^{90} + 6x^{128} \\ &+ (12n-12)x^{144} + (24n-24)x^{180} + (54n^2-114n+60)x^{200}. \end{aligned}$$

□

4. Results for Regular Triangulate Oxide Network $RTOX(n)$

In this section, we consider a family of regular triangular oxide network which is denoted by $RTOX(n), n \geq 3$. The graph $RTOX(5)$, is shown in Figure 6.

Let G be the graph of $RTOX(n)$. The graph regular triangular oxide network $RTOX(n)$ has $3n^2+6n$ edges. Also there are three types of edges in G based on the degrees of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) | d_G(u) = d_G(v) = 2\}$, $|E_1| = 2$,
$E_2 = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 4\}$, $|E_2| = 6n$,
$E_3 = \{uv \in E(G) | d_G(u) = d_G(v) = 4\}$, $|E_3| = 3n^2 - 2$.

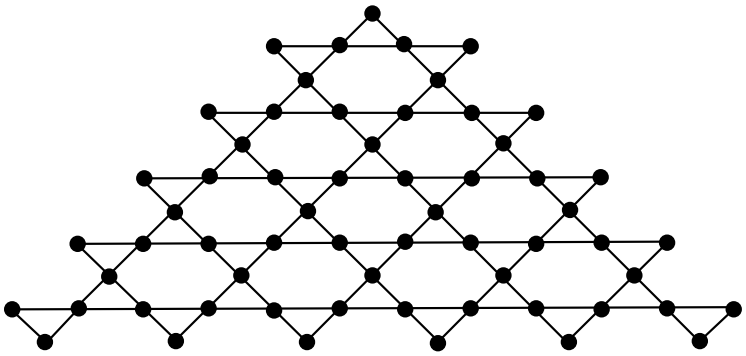

Figure 6: Regular triangular oxide network, $RTOX(5)$.

The partition of the edges with respect to their sum degree of end vertices of regular triangular oxide network is given in Table 5.

Table 5: Edge partition of regular triangular oxide network $RTOX(n)$.

$(S_G[u], S_G[v]) \backslash uv \in E(G)$	Number of edges
$(8,8)$	2
$(8,16)$	4
$(10,16)$	4
$(10,18)$	$6n-8$
$(16,16)$	1
$(16,18)$	6
$(18,18)$	$6n-9$
$(18,20)$	$6n-12$
$(20,20)$	$3n^2-12n+12$

In the following theorems, we obtain explicit formulae for computing $BM_2(G)$, $BM_4(G)$, $BM_2(G,x)$ and $BM_4(G,x)$ of the regular triangular oxide network $RTOX(n)$.

Theorem 4.1. *Let $RTOX(n)$ be the family of regular triangular oxide network. Then*

1. $BM_2(RTOX(n)) = 600n^2 + 192n - 306$.
2. $BM_4(RTOX(n)) = 120000n^2 - 79536n - 24964$.

Proof. We give the proof for one of the topological graph indices under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 5. Then

$$\begin{aligned}
BM_2(G) &= \sum_{uv\in E(G)} \frac{S_G[u]S_G[v]}{2} \\
&= m_{8,8}\left(\frac{8\times 8}{2}\right) + m_{8,16}\left(\frac{8\times 16}{2}\right) + m_{10,16}\left(\frac{10\times 16}{2}\right) \\
&+ m_{10,18}\left(\frac{10\times 18}{2}\right) + m_{16,16}\left(\frac{16\times 16}{2}\right) + m_{16,18}\left(\frac{16\times 18}{2}\right) \\
&+ m_{18,18}\left(\frac{18\times 18}{2}\right) + m_{18,20}\left(\frac{18\times 20}{2}\right) + m_{20,20}\left(\frac{20\times 20}{2}\right) \\
&= 600n^2 + 192n - 306.
\end{aligned}$$

□

Theorem 4.2. *Let $RTOX(n)$ be the family of regular triangular oxide network. Then*

1. $BM_2(RTOX(n),x) = 2x^{32} + 4x^{64} + 4x^{80} + (6n-8)x^{90} + x^{128} + 6x^{144} + (6n-9)x^{162} + (6n-12)x^{180} + (3n^2-12n+12)x^{200}$.
2. $BM_4(RTOX(n),x) = 2x^{1024} + 4x^{4096} + 4x^{6400} + (6n-8)x^{8100} + x^{16384} + 6x^{20736} + (6n-9)x^{26244} + (6n-12)x^{32400} + (3n^2-12n+12)x^{40000}$.

Proof. We give the proof for one of the topological graph polynomial under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 5. Then

$$\begin{aligned}
BM_2(G,x) &= \sum_{uv\in E(G)} x^{\frac{S_G[u]S_G[v]}{2}} \\
&= m_{8,8}x^{\left(\frac{8\times 8}{2}\right)} + m_{8,16}x^{\left(\frac{8\times 16}{2}\right)} + m_{10,16}x^{\left(\frac{10\times 16}{2}\right)} \\
&+ m_{10,18}x^{\left(\frac{10\times 18}{2}\right)} + m_{16,16}x^{\left(\frac{16\times 16}{2}\right)} + m_{16,18}x^{\left(\frac{16\times 18}{2}\right)} \\
&+ m_{18,18}x^{\left(\frac{18\times 18}{2}\right)} + m_{18,20}x^{\left(\frac{18\times 20}{2}\right)} + m_{20,20}x^{\left(\frac{20\times 20}{2}\right)} \\
&= 2x^{32} + 4x^{64} + 4x^{80} + (6n-8)x^{90} + x^{128} + 6x^{144} \\
&+ (6n-9)x^{162} + (6n-12)x^{180} + (3n^2-12n+12)x^{200}.
\end{aligned}$$

□

5. Results for H-Naphtalenic nanotubes

In this section, we consider a family of H-Naphtalenic nanotubes. This nanotube is a trivalent decoration having a sequence of $C_6, C_6, C_4, C_6, C_6, C_4, ...$ in the first row and a sequence of $C_6, C_8, C_6, C_8, ...$ in other row. This nanotube is denoted by $NHPX[m, n]$, where m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as shown in Figure 7.

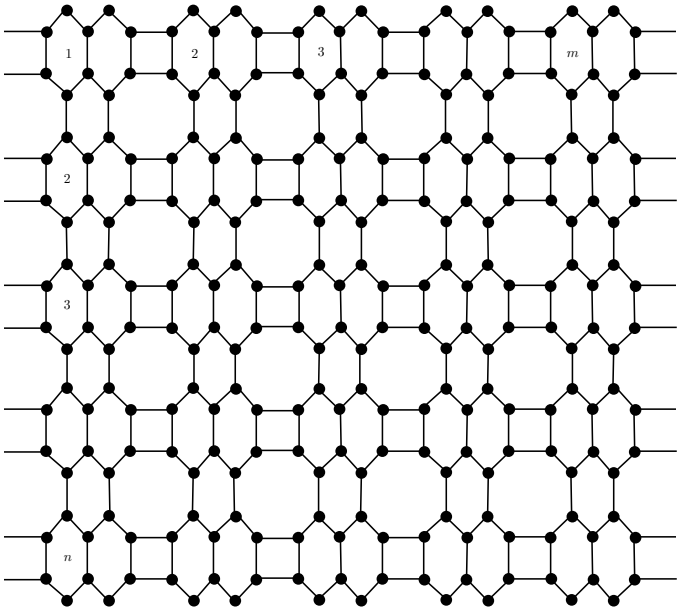

Figure 7: H-Naphtalenic nanotubes $NHPX[m, n]$.

Let G be the graph of a nanotube $NHPX[m, n]$. The graph H-Naphtalenic nanotubes $NHPX[m, n]$ has $15mn - 2m$ edges. Also there are two types of edges in G based on the degrees of end vertices of each edge as follows:

$$E_1 = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 3\}, \qquad |E_1| = 8m,$$
$$E_2 = \{uv \in E(G) | d_G(u) = d_G(v) = 3\}, \qquad |E_2| = 15mn - 10m$$

The partition of the edges with respect to their sum degree of end vertices of H-Naphtalenic nanotubes is given in Table 6.

Table 6: Edge partition of H-Naphtalenic nanotubes $NHPX[m, n]$.

$(S_G[u], S_G[v])$	(8, 10)	(8, 11)	(11, 11)	(10, 12)	(11, 12)	(12, 12)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn - 18m$

In the following theorems, we obtain explicit formulae for computing $BM_2(G)$, $BM_4(G)$, $BM_2(G, x)$ and $BM_4(G, x)$ of the H-Naphtalenic nanotubes $NHPX[m, n]$.

Theorem 5.1. *Let $NHPX[m, n]$ be the family of H-Naphtalenic nanotubes. Then*

1. $BM_2(NHPX[m, n]) = 1080mn - 455m$.
2. $BM_4(NHPX[m, n]) = 77760mn - 47223.5m$.

Proof. We give the proof for one of the topological graph indices under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 6. Then

$$\begin{aligned} BM_2(G) &= \sum_{uv\in E(G)} \frac{S_G[u]S_G[v]}{2} \\ &= m_{8,10}\left(\frac{8\times 10}{2}\right) + m_{8,11}\left(\frac{8\times 11}{2}\right) + m_{11,11}\left(\frac{11\times 11}{2}\right) \\ &+ m_{10,12}\left(\frac{10\times 12}{2}\right) + m_{11,12}\left(\frac{11\times 12}{2}\right) + m_{12,12}\left(\frac{12\times 12}{2}\right) \\ &= 1080mn - 455m. \end{aligned}$$

□

Theorem 5.2. *Let $NHPX[m,n]$ be the family of H-Naphtalenic nanotubes. Then*

1. $BM_2(NHPX[m,n],x) = 4mx^{40} + 4mx^{44} + 2mx^{\frac{121}{2}} + 2mx^{60} + 4mx^{66} + (15mn - 18m)x^{72}$.
2. $BM_4(NHPX[m,n],x) = 4mx^{1600} + 4mx^{1936} + 2mx^{\frac{14641}{4}} + 2mx^{3600} + 4mx^{4356} + (15mn - 18m)x^{5184}$.

Proof. We give the proof for one of the topological graph polynomial under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 6. Then

$$\begin{aligned} BM_2(G,x) &= \sum_{uv\in E(G)} x^{\frac{S_G[u]S_G[v]}{2}} \\ &= m_{8,10}x^{\left(\frac{8\times 10}{2}\right)} + m_{8,11}x^{\left(\frac{8\times 11}{2}\right)} + m_{11,11}x^{\left(\frac{11\times 11}{2}\right)} \\ &+ m_{10,12}x^{\left(\frac{10\times 12}{2}\right)} + m_{11,12}x^{\left(\frac{11\times 12}{2}\right)} + m_{12,12}x^{\left(\frac{12\times 12}{2}\right)} \\ &= 4mx^{40} + 4mx^{44} + 2mx^{\frac{121}{2}} + 2mx^{60} + 4mx^{66} + (15mn - 18m)x^{72}. \end{aligned}$$

□

6. Results for Nanocones $C_n[k]$

In this section, we consider nanocones $C_n[k]$. The molecular structure of $C_2[4]$ is shown in Figure 8.

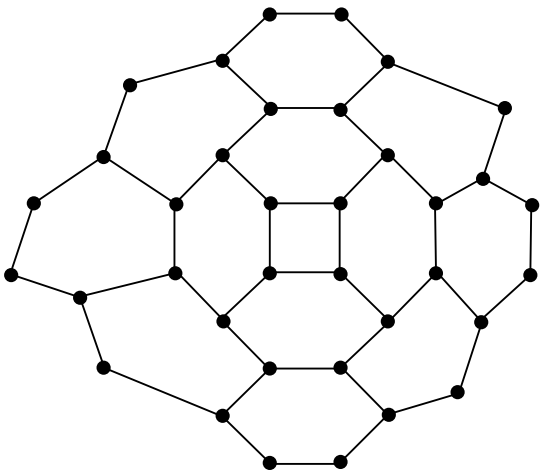

Figure 8: Molecular structure of Nanocone $C_2[4]$

Let G be the molecular structure of $C_n[k]$. The graph molecular structure of $C_n[k]$ has $n(k+1)^2$ vertices and $\frac{3}{2}nk^2+\frac{5}{2}nk+n$ edges. Also there are three types of edges in G based on the degrees of end vertices of each edge as follows:

$$\begin{array}{ll} E_1=\{uv\in E(G)|d_G(u)=d_G(v)=2\}, & |E_1|=n,\\ E_2=\{uv\in E(G)|d_G(u)=2,d_G(v)=3\}, & |E_2|=2nk,\\ E_3=\{uv\in E(G)|d_G(u)=d_G(v)=3\}, & |E_3|=\frac{3}{2}nk^2+\frac{1}{2}nk, \end{array}$$

The partition of the edges with respect to their sum degree of end vertices of molecular structure of $C_n[k]$ nanocones is given in Table 7.

Table 7: Edge partition of molecular structure of $C_n[k]$ nanocones.

$(S_G[u],S_G[v])$	(7, 7)	(7, 10)	(8, 10)	(10, 12)	(12, 12)
Number of edges	n	$2n$	$2(k-1)n$	nk	$\frac{nk}{2}(3k-1)$

In the following theorems, we obtain explicit formulae for computing $BM_2(G)$, $BM_4(G)$, $BM_2(G,x)$ and $BM_4(G,x)$ of the molecular structure of $C_n[k]$ nanocones.

Theorem 6.1. *Let $C_n[k]$ be the family of nanocones. Then*

1. $BM_2(C_n[k])=108nk^2+104nk+14.5n$.
2. $BM_4(C_n[k])=7776nk^2+4208nk-149.75n$.

Proof. We give the proof for one of the topological graph indices under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 7. Then

$$\begin{aligned} BM_2(G) &= \sum_{uv\in E(G)}\frac{S_G[u]S_G[v]}{2}\\ &= m_{7,7}\left(\frac{7\times 7}{2}\right)+m_{7,10}\left(\frac{7\times 10}{2}\right)+m_{8,10}\left(\frac{8\times 10}{2}\right)\\ &+ m_{10,12}\left(\frac{10\times 12}{2}\right)+m_{12,12}\left(\frac{12\times 12}{2}\right)\\ &= 108nk^2+104nk+14.5n. \end{aligned}$$

□

Theorem 6.2. *Let $C_n[k]$ be the family of nanocones. Then*

1. $BM_2(C_n[k],x)=nx^{\frac{49}{2}}+2nx^{35}+2(k-1)nx^{40}+nkx^{60}+\frac{nk}{2}(3k-1)x^{72}$.
2. $BM_4(C_n[k],x)=nx^{\frac{2401}{4}}+2nx^{1225}+2(k-1)nx^{1600}+nkx^{3600}+\frac{nk}{2}(3k-1)x^{5184}$.

Proof. We give the proof for one of the topological graph polynomial under consideration as the other follow the same reasoning after the edge partitions. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees $S_G[u]$ and $S_G[v]$. The number of edges in each row are listed in Table 7. Then

$$\begin{aligned} BM_2(G,x) &= \sum_{uv\in E(G)}x^{\frac{S_G[u]S_G[v]}{2}}\\ &= m_{7,7}x^{\left(\frac{7\times 7}{2}\right)}+m_{7,10}x^{\left(\frac{7\times 10}{2}\right)}+m_{8,10}x^{\left(\frac{8\times 10}{2}\right)}+m_{10,12}x^{\left(\frac{10\times 12}{2}\right)}+m_{12,12}x^{\left(\frac{12\times 12}{2}\right)}\\ &= nx^{\frac{49}{2}}+2nx^{35}+2(k-1)nx^{40}+nkx^{60}+\frac{nk}{2}(3k-1)x^{72}. \end{aligned}$$

□

7. Conclusion

In this paper, we have introduced a closed neighbourhood indices namely $BM_2(G)$ and $BM_4(G)$ indices and also $BM_2(G,x)$ and $BM_4(G,x)$ polynomials in the field of mathematical chemistry, it has chemical applicability in determining several physico-chemical properties of octane isomers as it has coefficient of correlation closer to 1, which is far better than other indices. Specially, $BM_2(G)$ and $BM_4(G)$ indices highly correlates with acentric factor (coefficient of correlation 0.9906546 and 0.9783643). Next, we have obtained $BM_2(G)$, $BM_4(G)$ indices and $BM_2(G,x)$, $BM_4(G,x)$ polynomials of dominating oxide network, regular triangulate oxide network, H-Naphtalenic nanotubes and nanocones of molecular graphs. Further, one can obtain different degree based indices of closed neighbourhood indices for chemical graphs.

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